Hard Probes
Asilomar Conference Grounds - Pacific Grove
12 June 2006

Heavy quark production: ~~theory~~

How well does leading twist pQCD really fare?

Matteo Cacciari
LPTHE - Paris 6

Outline

- What can be calculated in perturbative QCD
- How accurately we can/do calculate it? What tools are available?
- Does it work? Comparisons with data
- Implications for RHIC

NB. The purpose of this talk is to assess the situation of 'standard' pQCD calculations only. Dense matter effects are ignored

A generic heavy quark production process

NB. Already making some simplifications by splitting the process this way. More on this later.

$$pp \xrightarrow{pQCD} Q \xrightarrow{NP\,fragm.} H_Q \xrightarrow{decay} e$$

A generic final state observable

This part is QCD.
How accurately can we predict it?
What ingredients do we need?

Simplifications

- Neglect multiple scattering, assume leading twist really leading at least for pp scattering, and try to get the **best possible perturbative prediction** for this process
- Restrict to collinear factorization and calculate as many perturbative orders as possible for the leading twist contribution
- Establish the accuracy of the calculation, make it a **baseline prediction** before moving to more complicate processes like pA and AA collisions

Factorization "theorem" for heavy quark hadroproduction

Collins, Soper, Sterman, Nucl. Phys. B263 (1986) 37

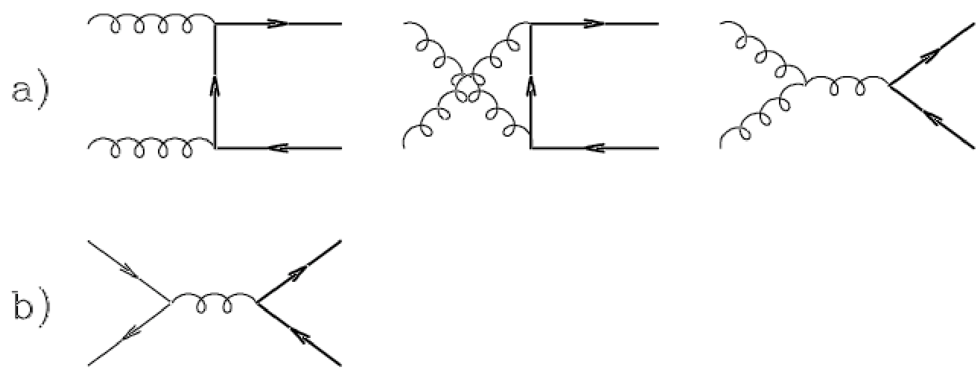
$$\sigma_Q(S,m^2) = \sum_{i,j\in L}\int dx_1 dx_2 \hat{\sigma}_{ij\to QX}(x_1x_2S, m^2; \alpha_s(\mu_R^2), \mu_R^2, \mu_F^2) F_{i/A}(x_1,\mu_F) F_{j/B}(x_2,\mu_F) + O\left(\frac{\Lambda}{m}\right)^p$$

Light flavours only

contribute most of the total cross section. The hard scattering function is perturbatively calculable in an expansion in powers of $\alpha_s(M)$: potential singularities in H have been factorized into the parton distribution functions. Corrections to this formula are suppressed by powers of (hadron mass scale/M).

We have by no means proved this result in this paper, but we believe that the analysis given here should make the result plausible. We are arguing that heavy

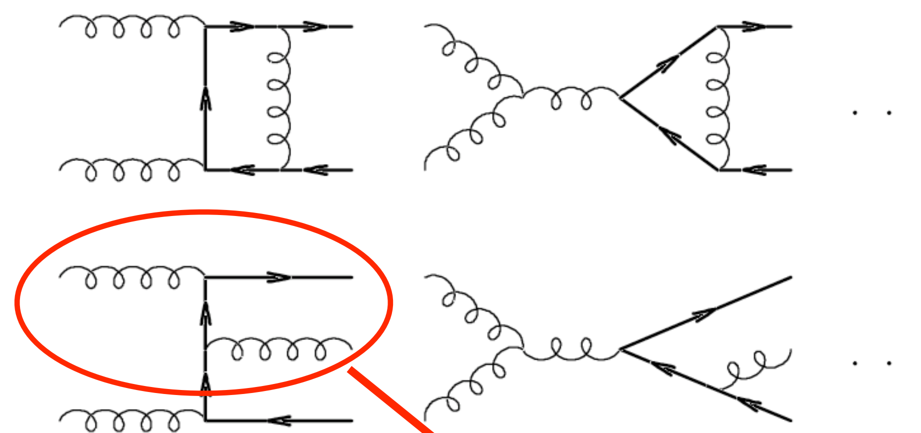
NLO implementation of factorization theorem



Leading order diagrams

(Some of the) Next-to-Leading order diagrams

Nason, Dawson, Ellis, NP B327 (1989) 49, NP B303 (1988) 607
Beenakker, van Neerven, Meng, Schuler, Smith, NP B351 (1991) 507



'flavour excitation'

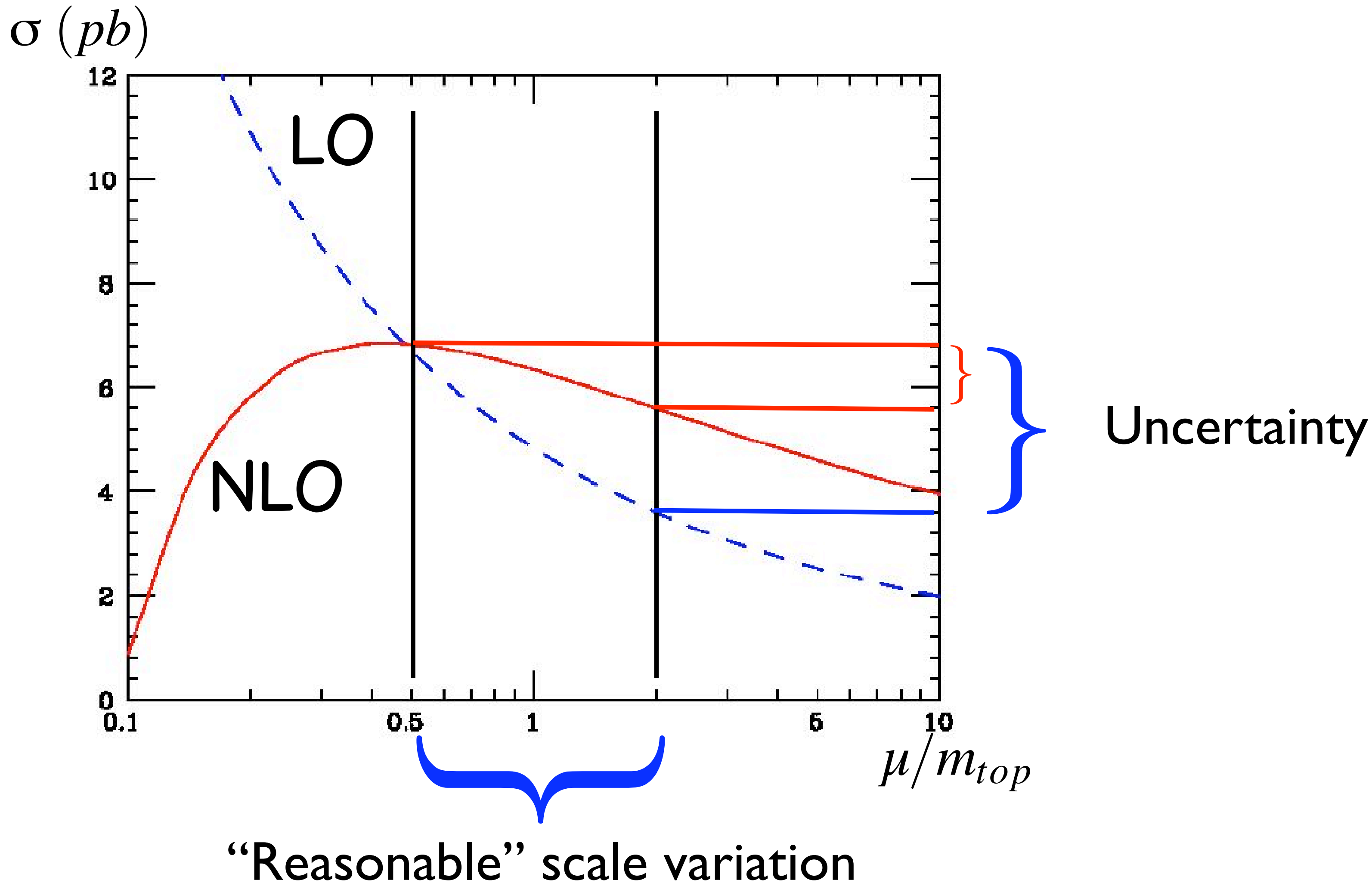
No need to have charm in the proton

This is still the state of the art for fixed order perturbative calculations, and should be the building block of all phenomenological predictions:

- it incorporates in a rigorous manner production "channels" like flavour excitation and gluon splitting which Monte Carlo or 'improved' leading order calculations have to include by hand (beware MC tunes and recipes!!)
- it allows a **rough estimate of the theoretical uncertainty**

The rule of thumb on uncertainties

“Typical” behaviour of a cross-section w.r.t. scale variations

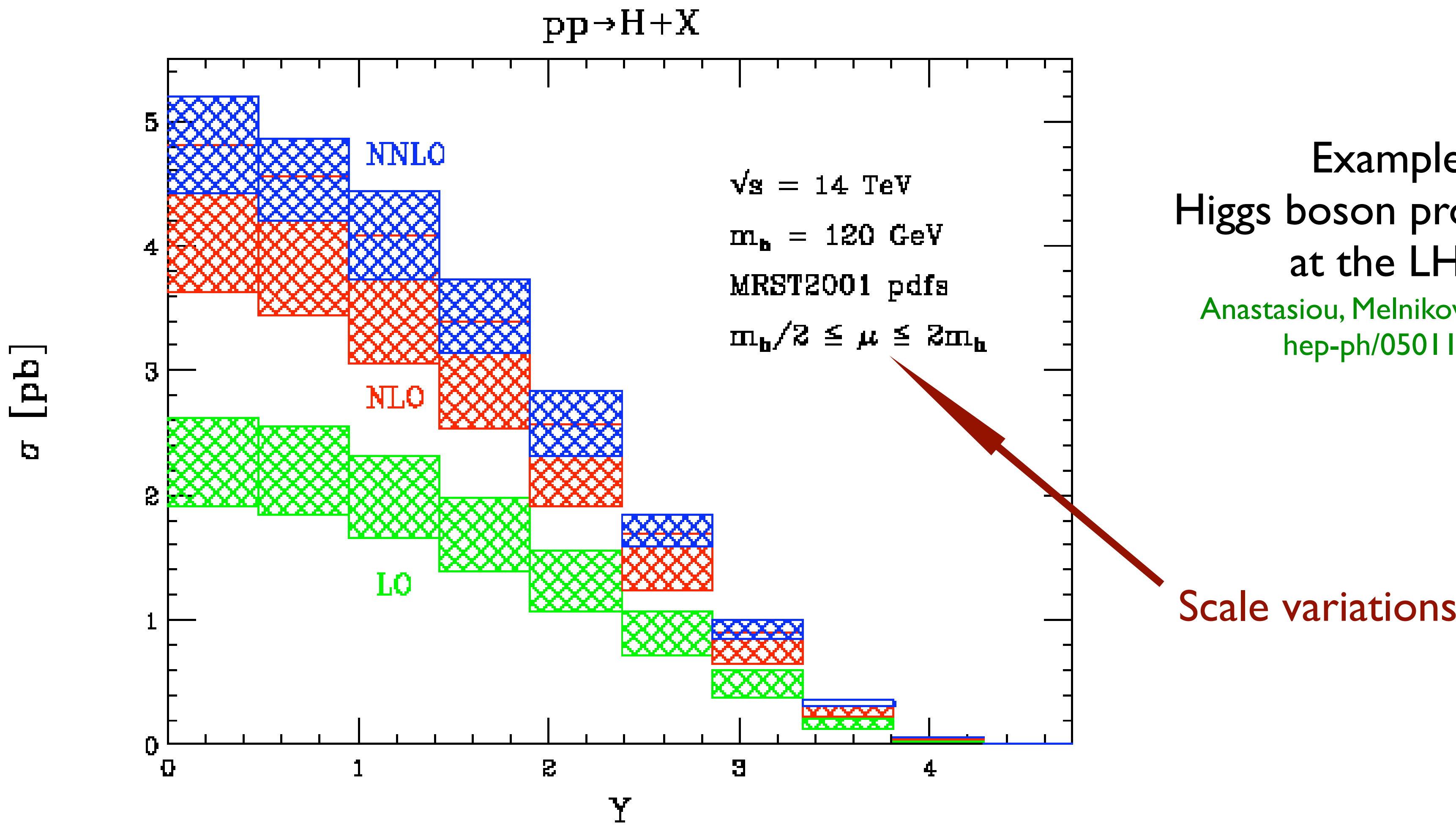


- A **LO** calculation gives you a **rough estimate** of the cross section

- A **NLO** calculation gives you a **good estimate** of the cross section and a **rough estimate** of the uncertainty

The rule of thumb on uncertainties

- A **NNLO** calculation gives you a **good estimate** of the uncertainty



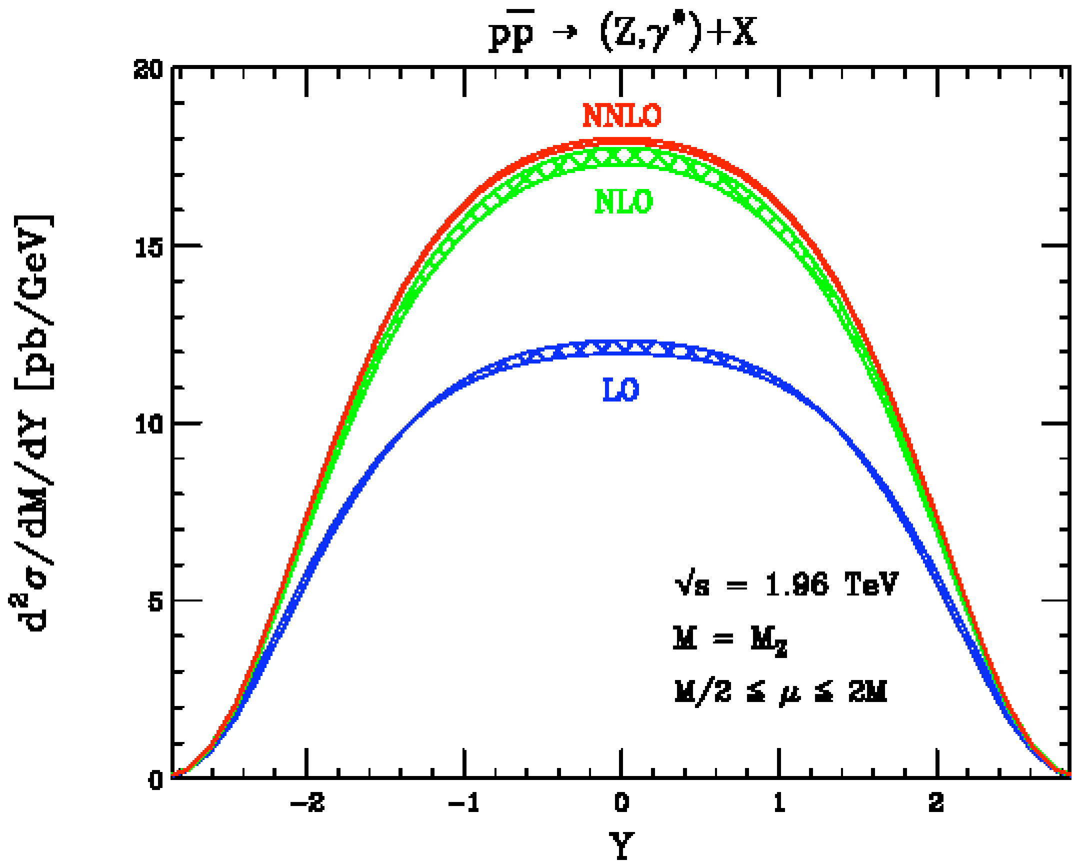
Example:
Higgs boson production
at the LHC
Anastasiou, Melnikov. Petriello,
hep-ph/05011030

NB. This example shows that the center of the NLO band has nothing to do with the most accurate theoretical prediction.

Theoretical uncertainty bands are not gaussian errors!

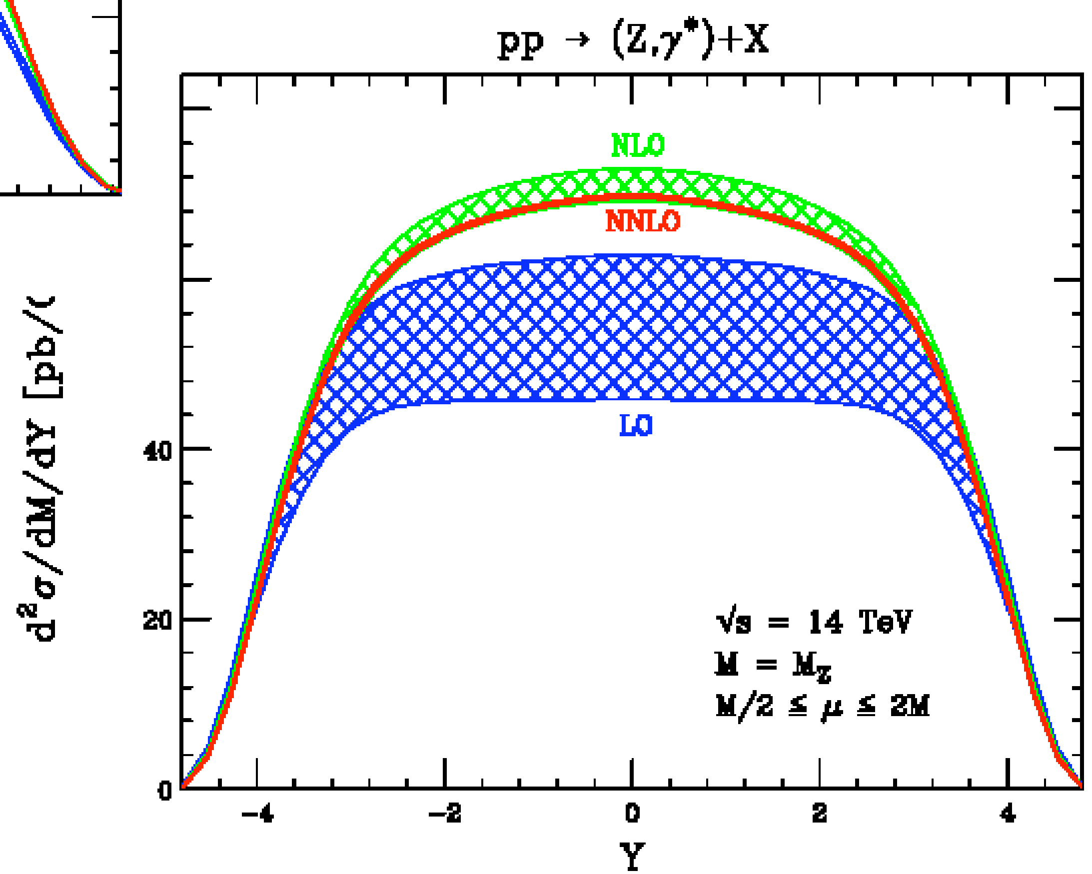
One more example

Anastasiou, Dixon, Melnikov. Petriello, hep-ph/0312266



Z production at the Tevatron

If you think you've found a standard rule, *"NNLO is on the upper limit of the NLO uncertainty band"*, think again



Z production at the LHC:
NNLO now on the lower side of the NLO uncertainty band

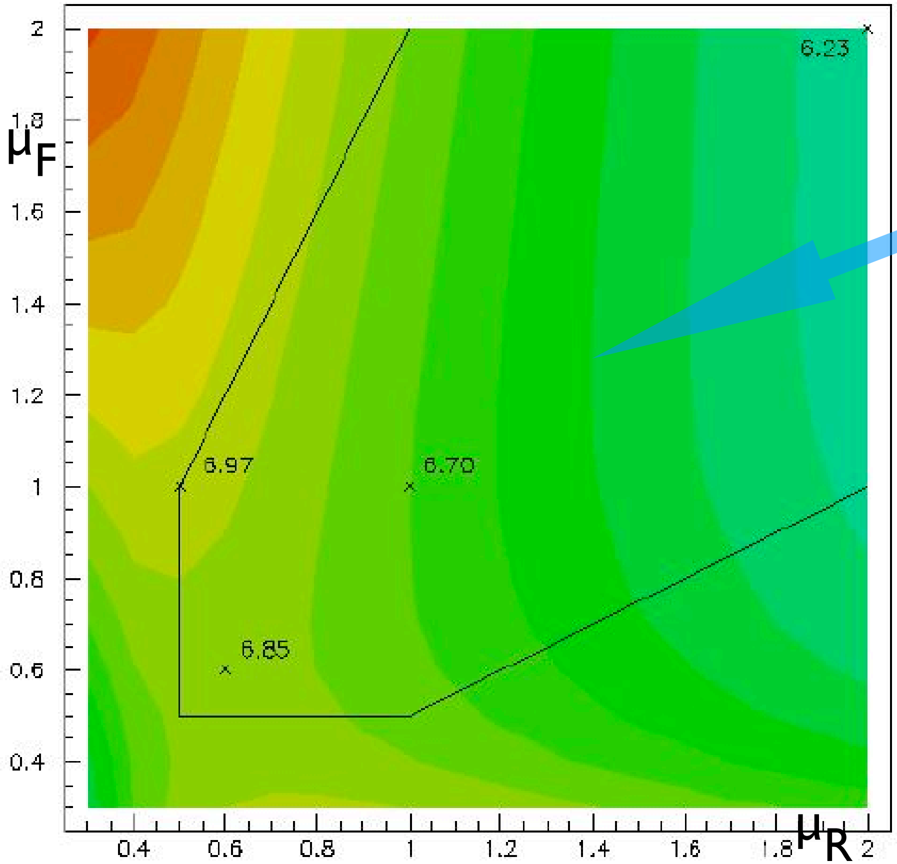
A theoretical *uncertainy band* is meant to be just that: you don't know where the higher order will be

Uncertainties estimate: top @ Tevatron

Standard procedure: vary renormalization and factorization scales.
But, better do so **independently**

σ: 6.82 > 6.70 > 6.23 pb $0.5 < \mu_{R,F}/m < 2$

σ: 6.97 > 6.70 > 6.23 pb $0.5 < \mu_{R,F}/m < 2$ && $0.5 < \mu_R/\mu_F < 2$

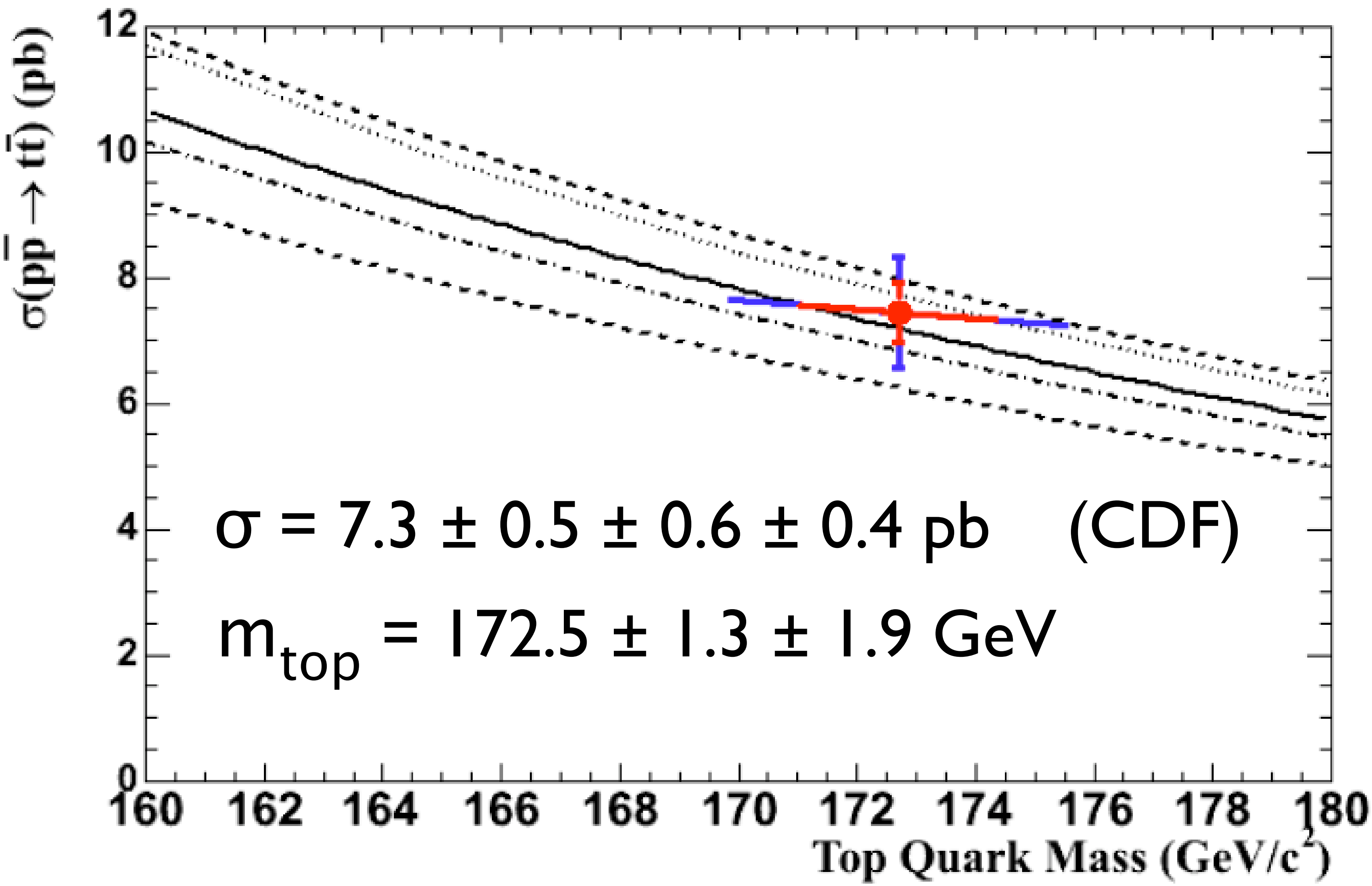


"Fiducial" region

Order **±5%** uncertainty along the diagonal, a little more when considering independent scale variations

NB. The PDF uncertainty (±10-15%) is the dominant one here

top @ Tevatron Run II



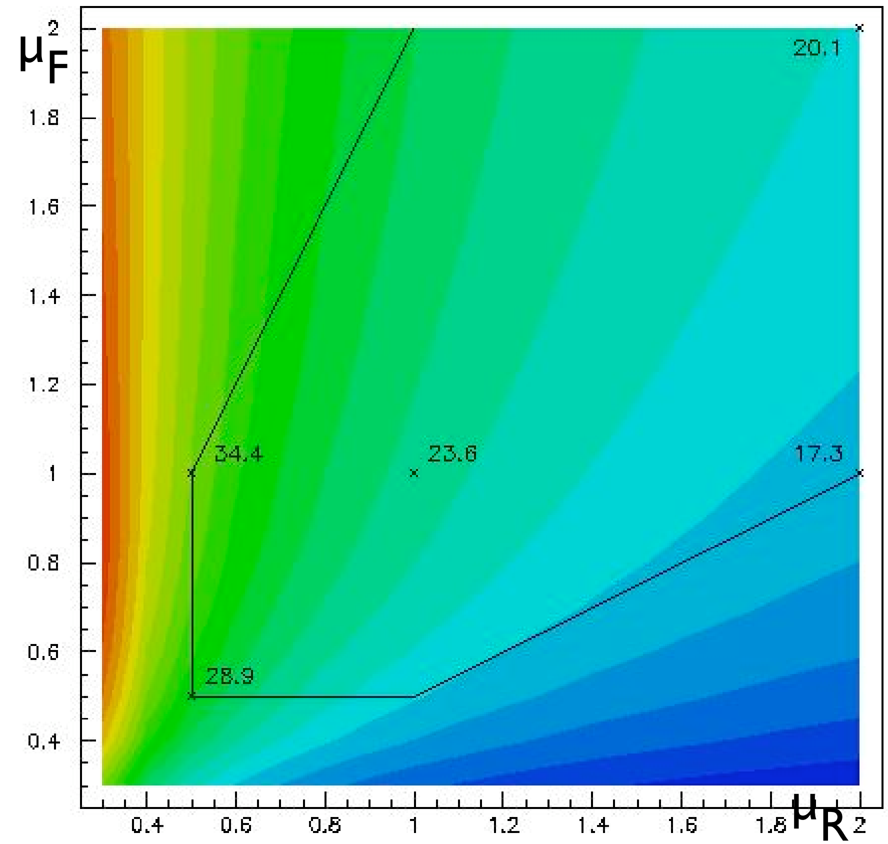
pQCD works perfectly here.
Experimental uncertainties now of the same order as the theoretical ones.

Uncertainties estimate: bottom @ Tevatron Run II

Scale uncertainties:

σ: 28.9 > 23.6 > 20.1 μb
$0.5 < \mu_{R,F}/\mu_0 < 2$

σ: 34.4 > 23.6 > 17.3 μb
$0.5 < \mu_{R,F}/\mu_0 < 2$ && $0.5 < \mu_R/\mu_F < 2$



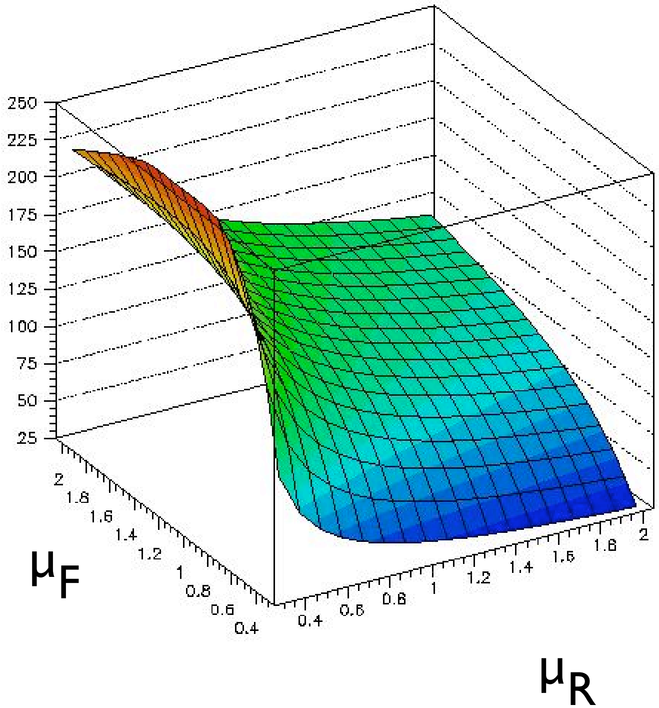
1) the scale uncertainties increase from **±18%** to **±35%** when going off-diagonal

2) PDF uncertainties are here less important than perturbative ones. At large p_T they become instead similar

Uncertainties estimate: bottom @ LHC

σ: 122 > 120 > 115 μb
$0.5 < \mu_{R,F}/\mu_0 < 2$

Only a **±4%** uncertainty when varying the scales together.......



σ: 178 > 120 > 75 μb
$0.5 < \mu_{R,F}/\mu_0 < 2$ && $0.5 < \mu_R/\mu_F < 2$

....which becomes a **±40%** one when going off-diagonal!

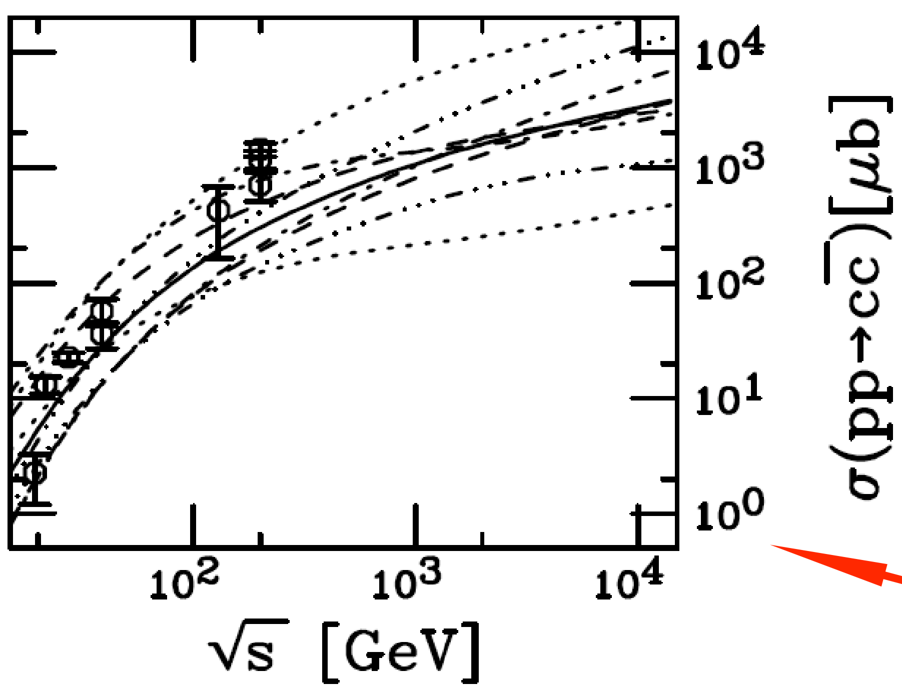
Note difference with Tevatron case. Not even the behaviour of uncertainties can be fully reliably extrapolated

Real observables

Total cross sections are rarely really measured

Often only a limited phase space region is available. These data can then be extrapolated to the full phace space.

This, of course, means adding the bias of a theoretical prejudice to an experimental measuremens



When the theoretical calculations are known to be accurate and precise and/or the extrapolation is small, there is no problem in doing so. Otherwise, we might end up with something closer to a theoretical estimate than to an experimental measurements.

Uncertainties for charm total cross section

Real observables

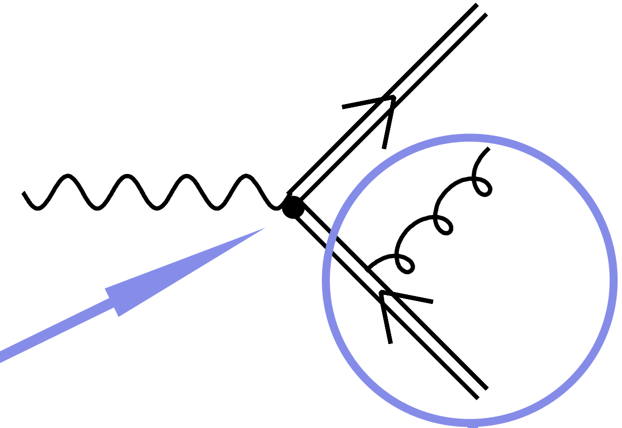
A safer solution is then to use differential observable quantities for comparing to theoretical predictions

Unfortunately, as usual, all good things come at a price:

Theoretical predictions for differential observables are **harder**

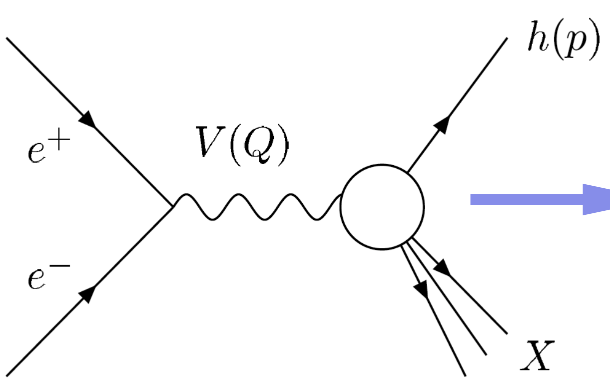
- Any multi-scale quantity in QCD will display possibly **large logarithms** in the perturbative expansion. These logs will tend to spoil the convergence of the series. Hence, **resummations** will be needed
- Eventually, resummations will not be enough, and genuinely **non-perturbative** contributions will need to be added

Heavy Quarks in e+e-

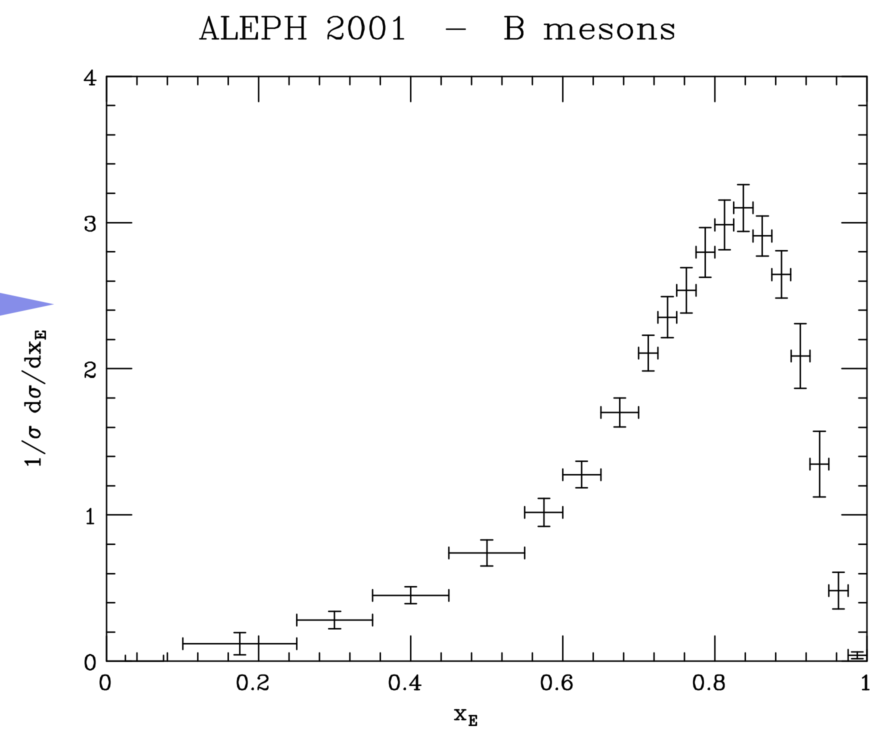


The Born level total production is of course an **electroweak** process

Fragmentation
is, instead, a QCD issue



$$x_E \equiv \frac{E_h}{E_{beam}}$$



At Born level x = 1. The momentum degradation of the heavy hadrons is a combination of **perturbative** and **non-perturbative** QCD effects

Perturbative Fragmentation

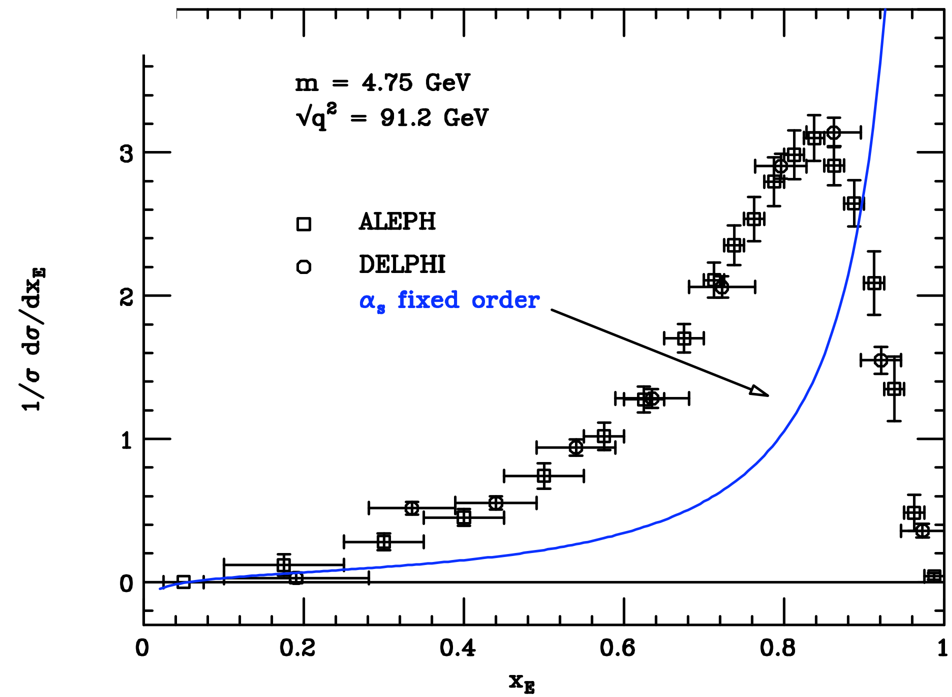
Collinear log

$$\frac{1}{\sigma}\frac{d\sigma}{dx} = \delta(1-x)+\frac{\alpha_s(Q^2)}{2\pi}\Big\{C_F+C_F\Big[\ln\frac{Q^2}{m^2}\left(\frac{1+x^2}{1-x}\right)_+ + 2\frac{1+x^2}{1-x}\log x - \left(\frac{\ln(1-x)}{1-x}\right)_+(1+x^2)+\frac{1}{2}\left(\frac{1}{1-x}\right)_+(x^2-6x-2) + \left(\frac{2}{3}\pi^2-\frac{5}{2}\right)\delta(1-x)\Big]\Big\} + \mathcal{O}\left(\frac{m}{Q}\right)$$

Soft logs

The LO calculation is a textbook example in QCD.
NB. Mass effects suppressed by the cms energy => negligible at LEP

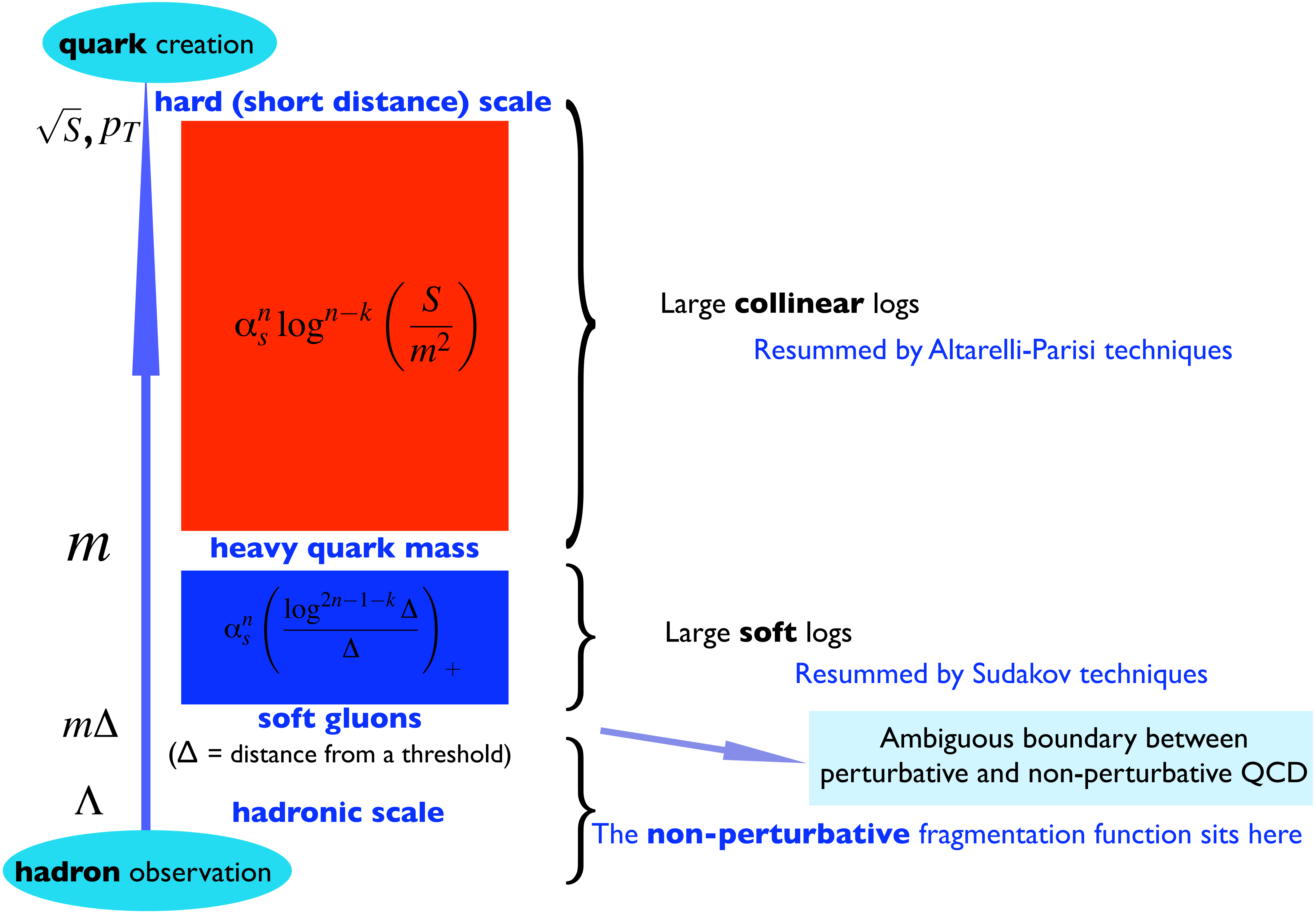
Comparison with experimental data is of course less than thrilling:



Two reasons for this:

- large **perturbative logs** spoil the convergence of the perturbative series
- significantly large **non-perturbative** contributions are missing

The many scales in heavy quark production



Resummation Tools

The state of the art for analytical theoretical predictions of heavy quark production is **Next-to-Leading Order** plus **Next-to-Leading Log** collinear resummation

This is usually implemented by taking

Fixed Order + Resummed - Double Counting

and usually returns single inclusive distributions

Alternatively, for more differential distributions, **MC@NLO** can be used.

Monte Carlo code by Frixione, Nason and Webber.
Interfaced with HERWIG, it is built so as to so merge a full **NLO calculation** with a **LL parton shower** and to avoid double counting

Advantages: NLO normalization and self-consistency built in.
No need for K-factors or recipes (one spoon of flavour excitation, two of gluon splitting, etc)

Non-perturbative fragmentation

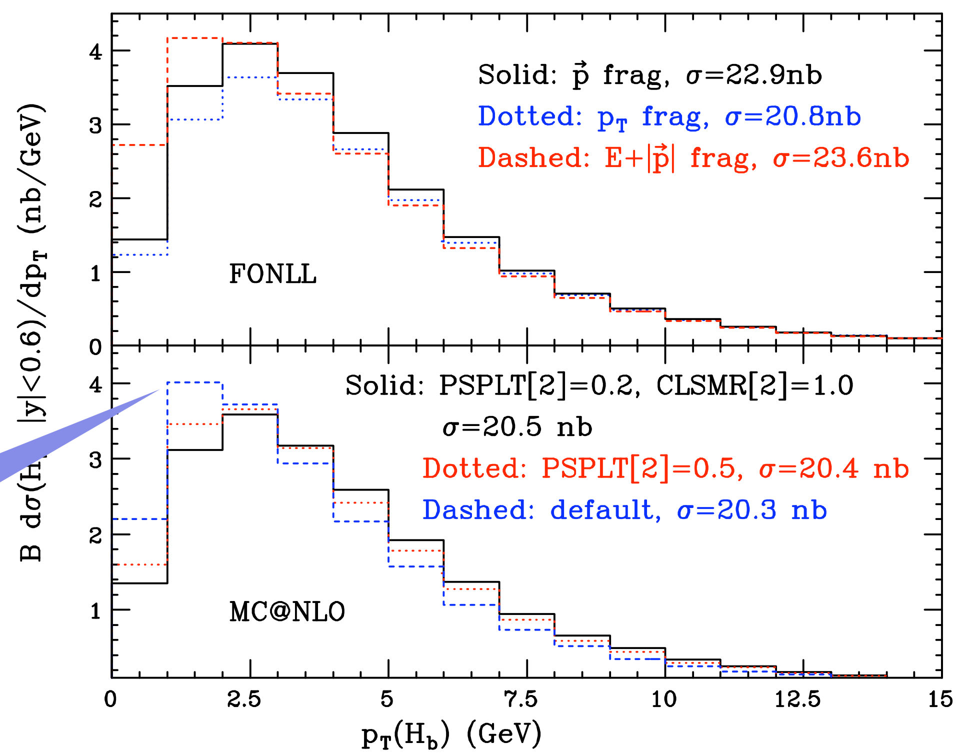
The non-perturbative FF is usually employed in hadronic collisions by writing

$$E_H \frac{d^3\sigma_H(p_H)}{dp_H^3} = E_Q \frac{d^3\sigma_Q(p_Q)}{dp_Q^3} \otimes D^{np}_{Q\to H}$$

Bear in mind that when the transverse momentum is small two things happen:

1. The "independent fragmentation" picture fails, as factorization-breaking higher twists grow large. So, whatever the result of the convolution above, there will be further uncertainties looming over it

2. Scaling a massive particle's 4-momentum is an ambiguous operation. One can scale the transverse momentum at constant rapidity, the 3-momentum at constant angle in a given frame, etc.

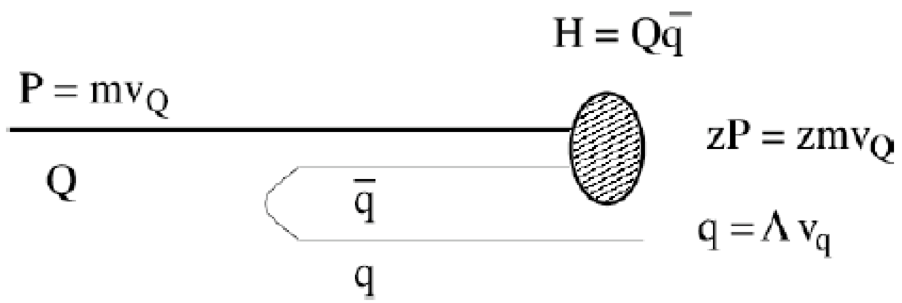


Different fragmentation choices

Non-perturbative Fragmentation

A heavy quark produced in a high energy event will lose a fraction of its momentum when picking up a light quark from the vacuum in order to hadronize into a heavy meson or baryon.

How much exactly we cannot tell (it's a non-perturbative process), but we can try to estimate it (more rigorous derivations are available):



The heavy quark has momentum $P = mv_Q$, the light quarks have momentum $q = \Lambda v_q$, with Λ a hadronic mass scale

For the binding we need $v_Q \simeq v_q = v$. We have then

$$P = zP + q \qquad\qquad mv = zmv + \Lambda v$$

and therefore

$$\langle z \rangle \simeq 1 - \frac{\Lambda}{m}$$

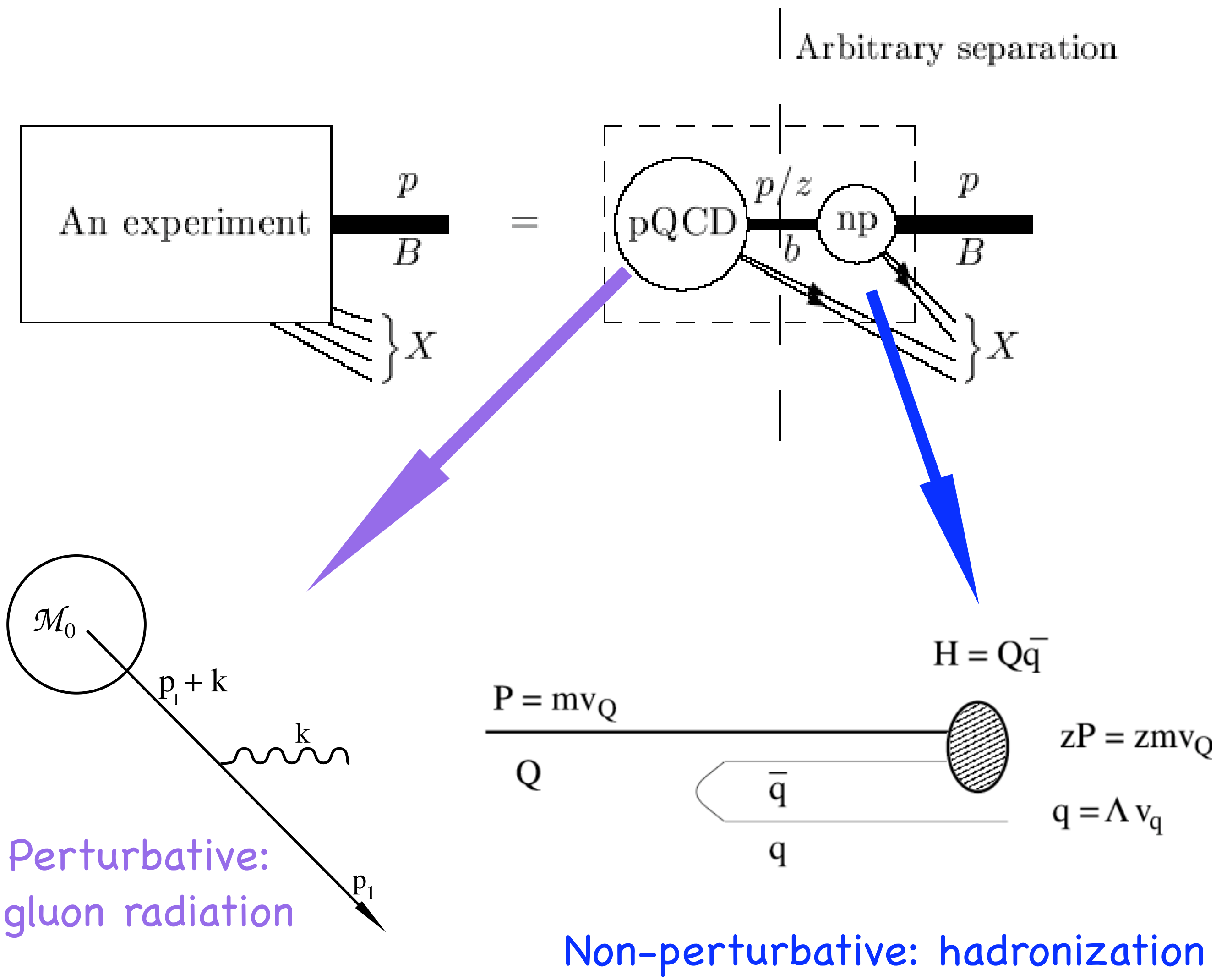
QCD predicts that the non-perturbative fragmentation of a heavy quark is very hard: the heavy quark loses a limited fraction of momentum (light hadron mass/heavy quark mass) when hadronising

This effect is far from negligible compared to the perturbative one. It usually parametrized by a **non-perturbative fragmentation function**, usually extracted from expt. data

No sensible phenomenology is possible without including non-perturbative contributions

Non-perturbative Fragmentation

When extracting the **heavy quark → heavy meson non-perturbative fragmentation function** from data, one must consider the **unavoidable interplay with perturbative physics**



Not being the c/b quark a physical particle, **the non-perturbative fragmentation function cannot be a physical observable**: its details depend on the perturbative calculation it is interfaced with.

A single fragmentation function cannot do for all calculations

Extraction of the non-perturbative component

Three issues are important:

1. The perturbative description (and its parameters) used in extracting the FF must match the one used in calculating predictions using the FF

2. Try to extract an as universal as possible non-perturbative FFs. Resumming the perturbative collinear logarithms (large at LEP: log(√S/m)) helps doing precisely this

3. Because of the steep slope of transverse momentum distributions in hadron-hadron collisions, higher Mellin moments of the FF are actually more important than its x-space shape:

Assuming $\frac{d\sigma}{d\hat{p}_T} \sim \frac{1}{\hat{p}_T^N}$ we get $\frac{d\sigma}{dp_T} \sim \int \frac{dz}{z} (\frac{z}{\hat{p}_T})^N f(z) = f_N \frac{d\sigma}{d\hat{p}_T}$

Heavy **quark** spectrum, N typically ~ 4,5

Heavy **meson** spectrum

Mellin **moment** of the fragmentation function

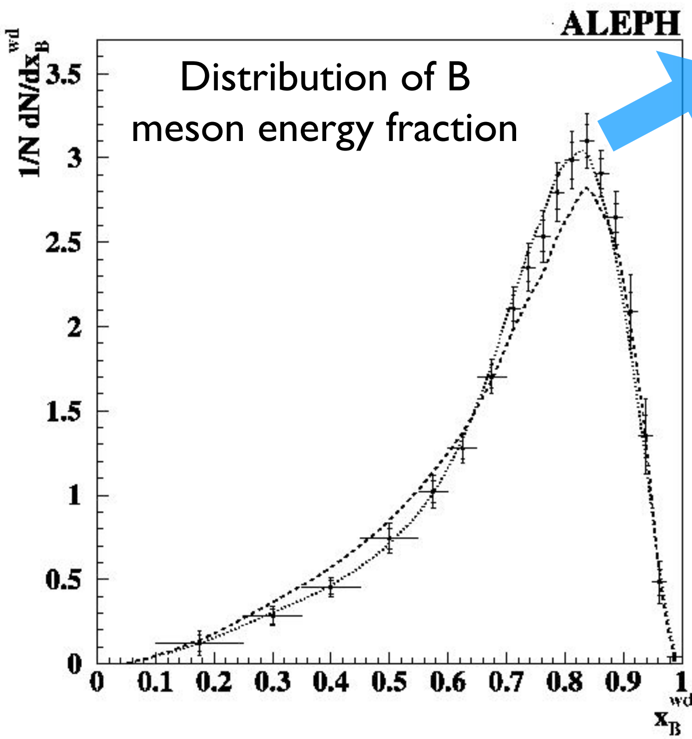
Heavy **quark** spectrum

Fitting well the proper moments (N ~ 4-5) is therefore more important then describing the whole fragmentation spectrum in e+e- collisions, if the fragmentation function is then to be used for making predictions in hadronic collisions

[This third step, is a bit exotheric, but numerically fairly important. It's the one which explaines why the usual Peterson FF in conjunction with a NLO calculation does not give a good description of heavy quark fragmentation: FF's extracted from moments are quite harder!]

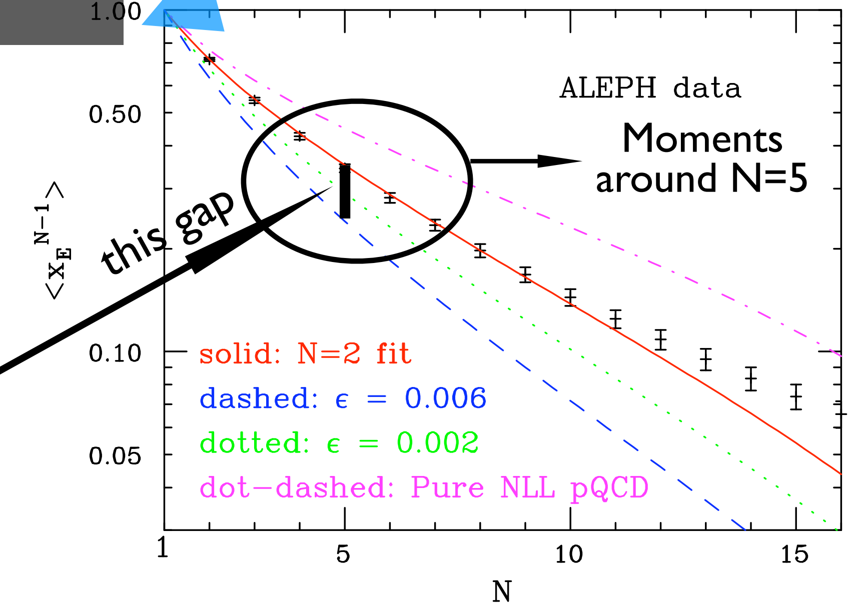
Extraction of the non-perturbative component for FONLL

Fit **moments** of LEP fragmentation data:



$$\langle x_E^{N-1} \rangle = \int_0^1 x_E^{N-1} f(x_E)\, dx_E$$

Note that Peterson with ϵ_b = 0.006 underestimates the moments around N=5. Its use will consequently underestimate the hadronic B cross section



Don’t fit this...... **...but rather this**

The extracted fragmentation functions are specific to the FONLL framework

For a comparison, they **roughly** correspond to Peterson et al. FF’s with $\boldsymbol{\epsilon_c \approx 0.005}$ and $\boldsymbol{\epsilon_b \approx 0.0005}$

⇒ quite harder than ‘usual’ values $\epsilon_c \approx 0.06$ and $\epsilon_b \approx 0.006$

⇒hadronic cross sections will be larger

Putting things together

A modern tool for producing phenomenological predictions for heavy quarks at the differential level will

1- properly **resum** (say to next-to-leading log accuracy) the large logarithms

2- **match** the resummation to a full NLO fixed order calculation

3- properly **extract** from data (and **use** for predictions) **non-perturbative** fragmentation functions describing the hadronization of the heavy quarks

NB. Whether you need all this or not depends, of course, on your accuracy goal. If you are happy with a factor of two uncertainties or more none of this is probably necessary: take the 15 years old NLO calculation and go ahead (but then don't come to me complaining of discrepancies with QCD!)

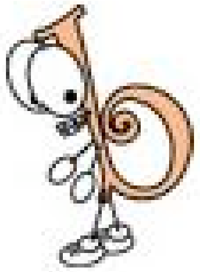
On the other hand, if you aim at a few 10% accuracy then you need this stuff.

Comparisons of phenomenological QCD predictions and experimental data

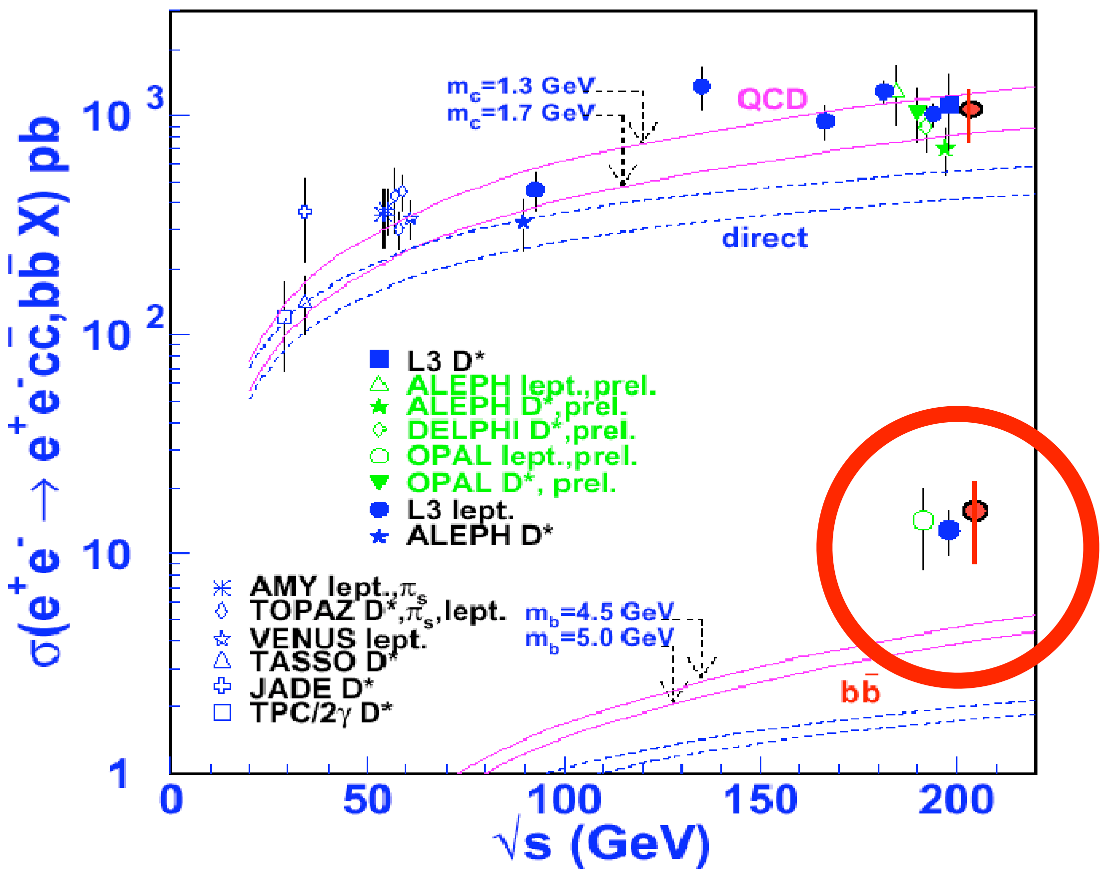
LEP, HERA, Tevatron, RHIC

Charm and Bottom

Bottom



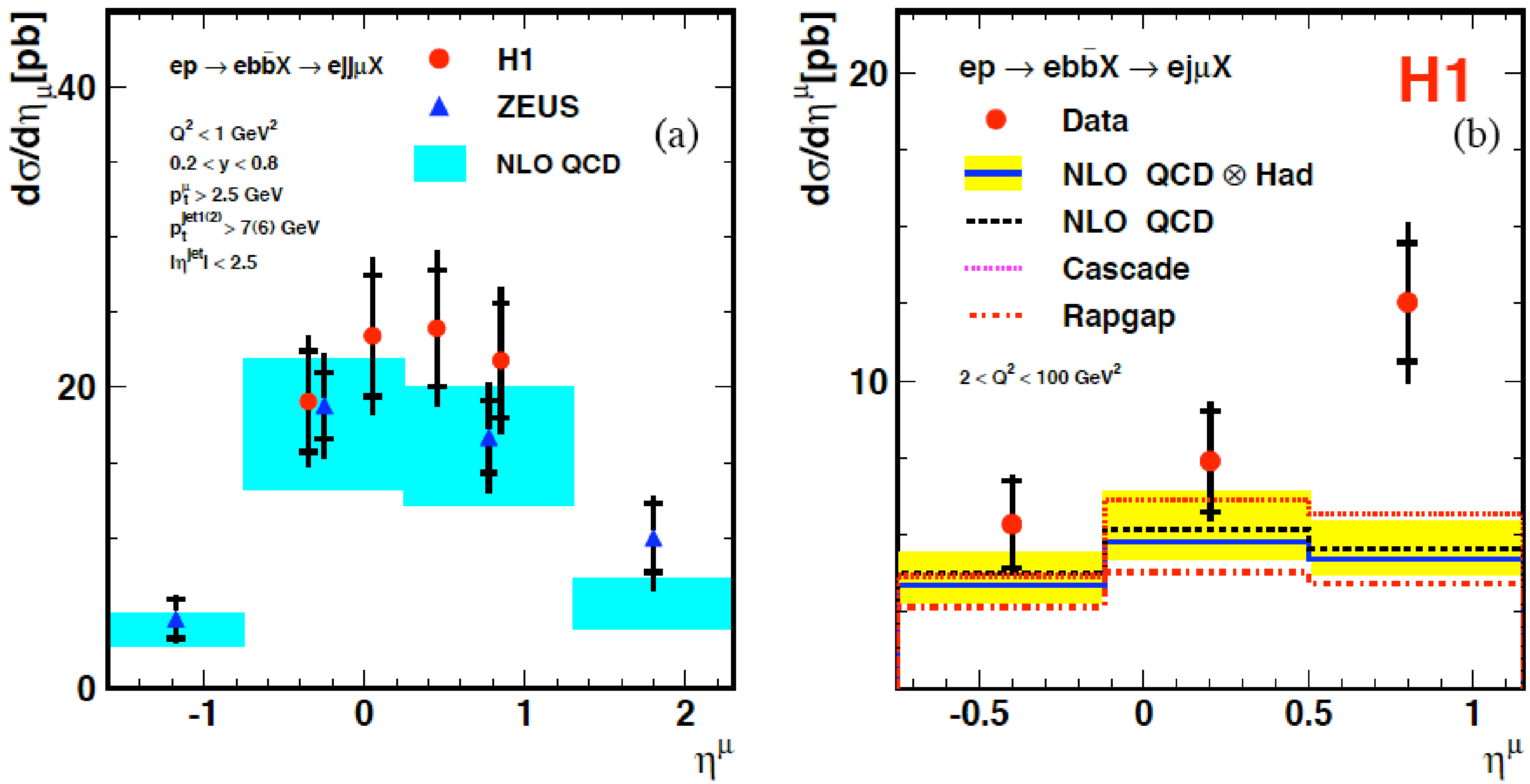
Bottom production @ LEP 2



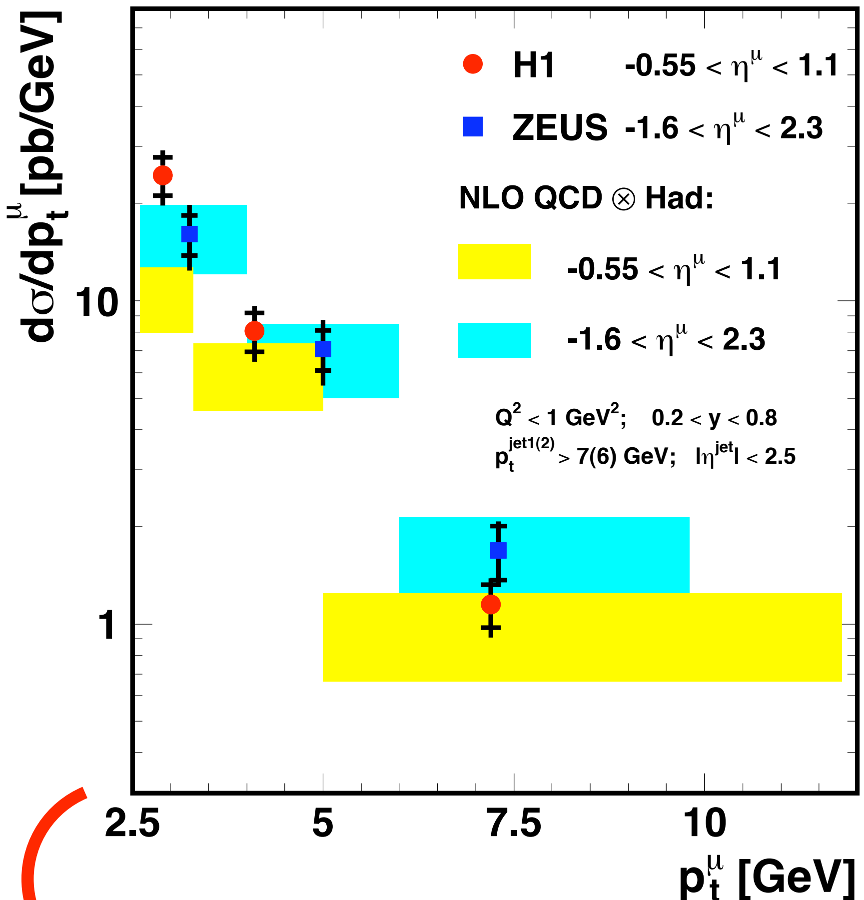
Worst alleged disagreement presently known (I think)

But.... data extrapolated to total cross section.
Not a real differential observable quantity (more differential distributions are available. Awaiting comparison with a theoretical calculation)

Bottom photoproduction @ HERA



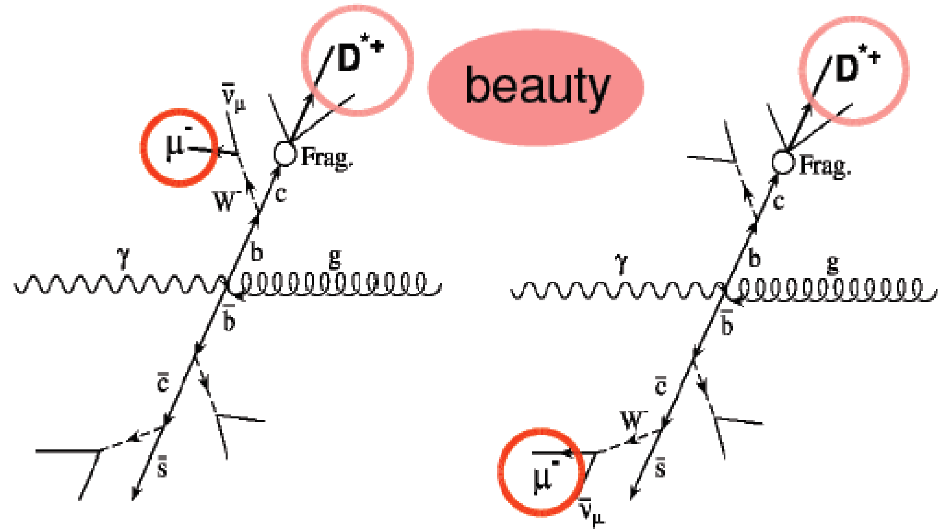
Bottom photoproduction @ HERA



ZEUS: No excess at low p_t^μ

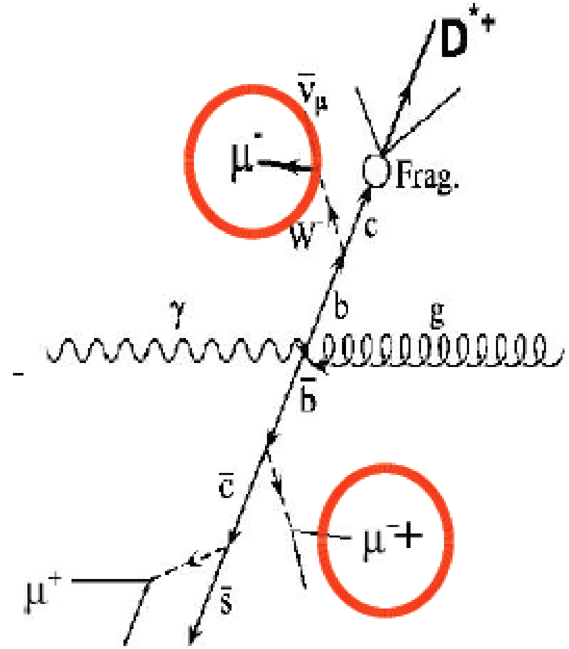
Bottom production @ HERA: D* + μ

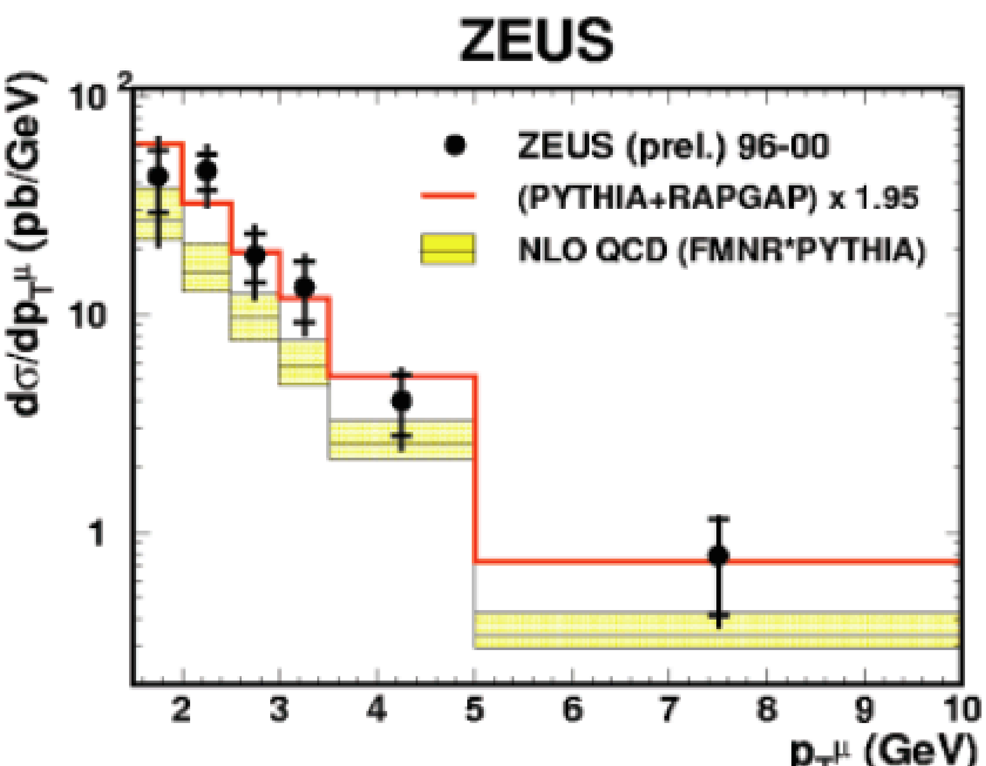
Data compared to NLO calculation (FMNR interfaced with PYTHIA)

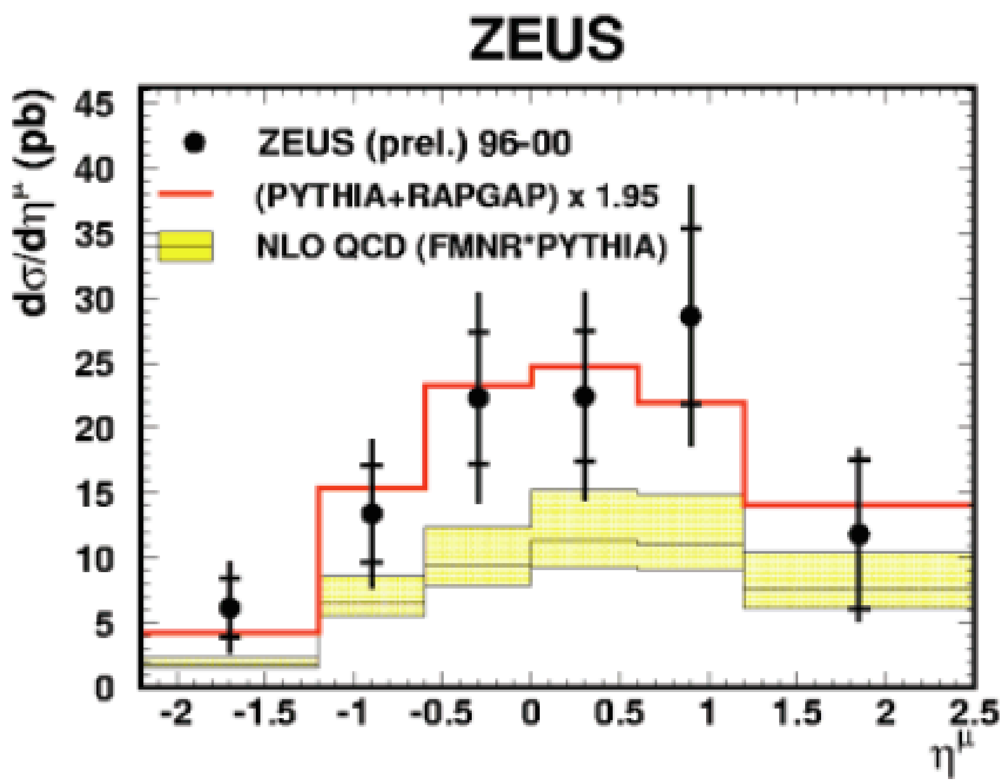


$p_T(D^*) > 1.9$ GeV, $-1.5 < \eta(D^*) < 1.5$, $p_T(\mu) > 1.4$ GeV, $-1.75 < \eta(\mu) < 1.3$	data/NLO
ZEUS $\sigma_{vis} = 214 \pm 52(\text{stat})\,^{+96}_{-84}\,(\text{syst.})$ pb FMNR⊗PYTHIA $\sigma_{vis} = 72\,^{+20}_{-13}\,(\text{NLO})\,^{+14}_{-10}$ pb	$3.1\,^{+1.6}_{-1.7}$
Photoproduction only: $Q^2<1$ GeV^2, $0.05<y<0.85$ ZEUS $\sigma_{vis} = 159 \pm 41(\text{stat})\,^{+68}_{-62}\,(\text{syst.})$ pb FMNR⊗PYTHIA $\sigma_{vis} = 57\,^{+16}_{-10}\,(\text{NLO})\,^{+11}_{-9}$ pb	$2.8\,^{+1.5}_{-1.6}$

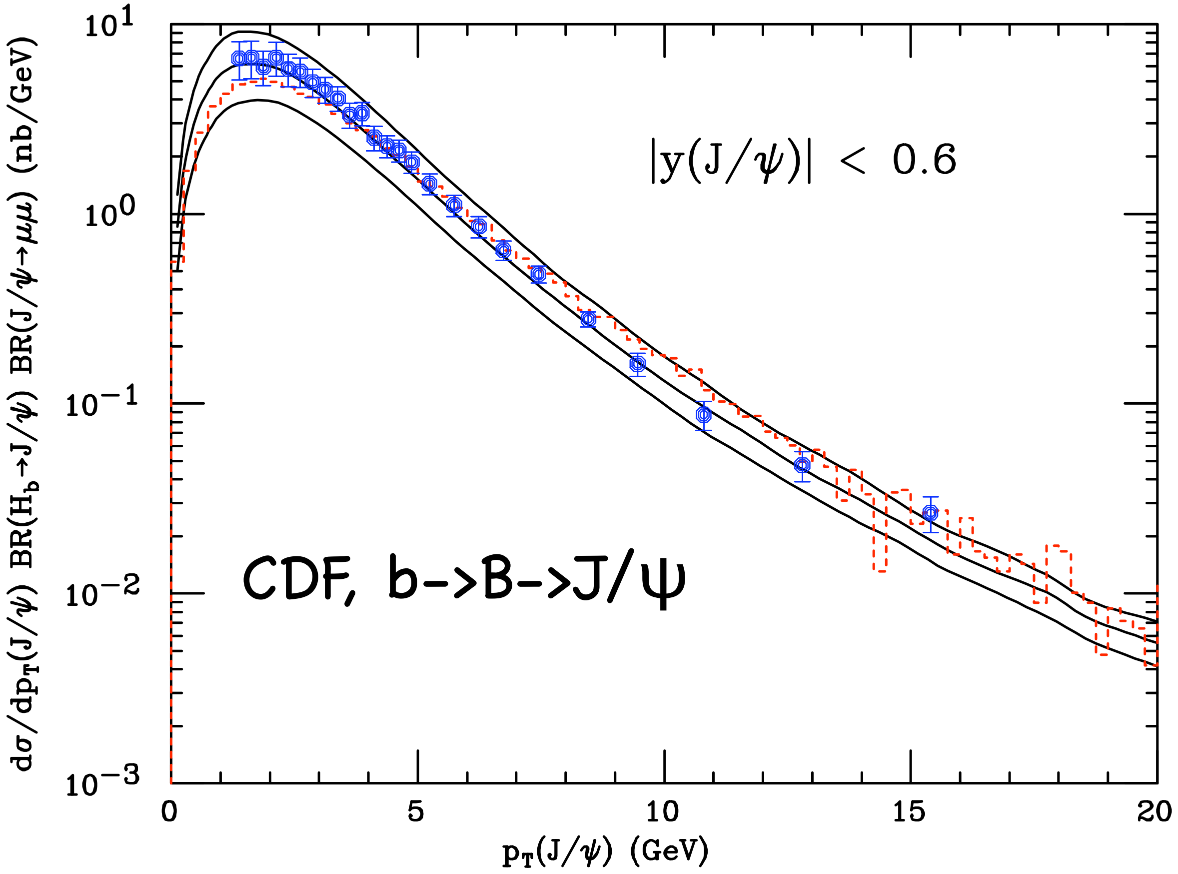
Bottom production @ HERA: μ+μ







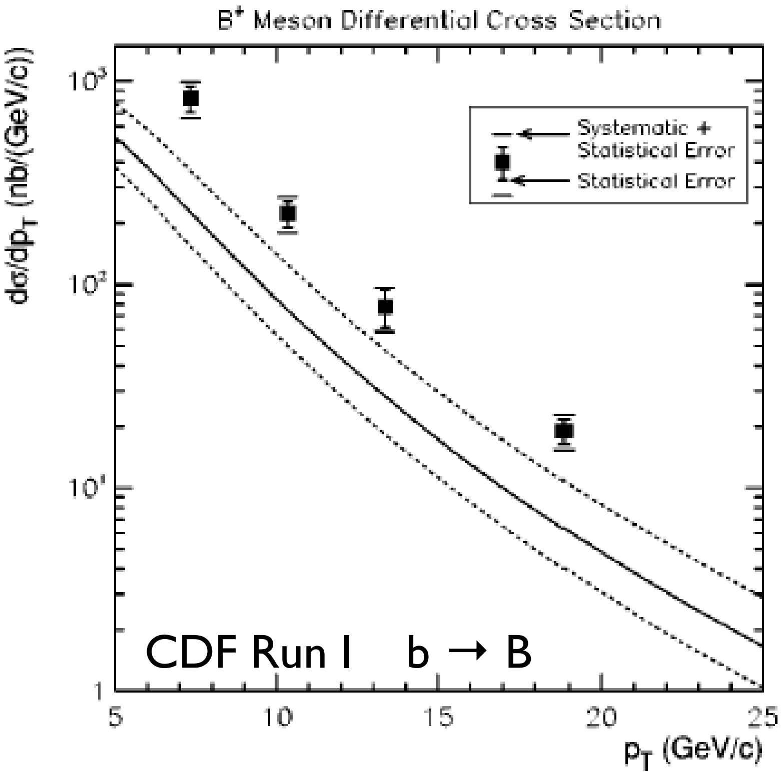
Bottom production @ Tevatron Run 2



Lines: FONLL
Histograms: MC@NLO

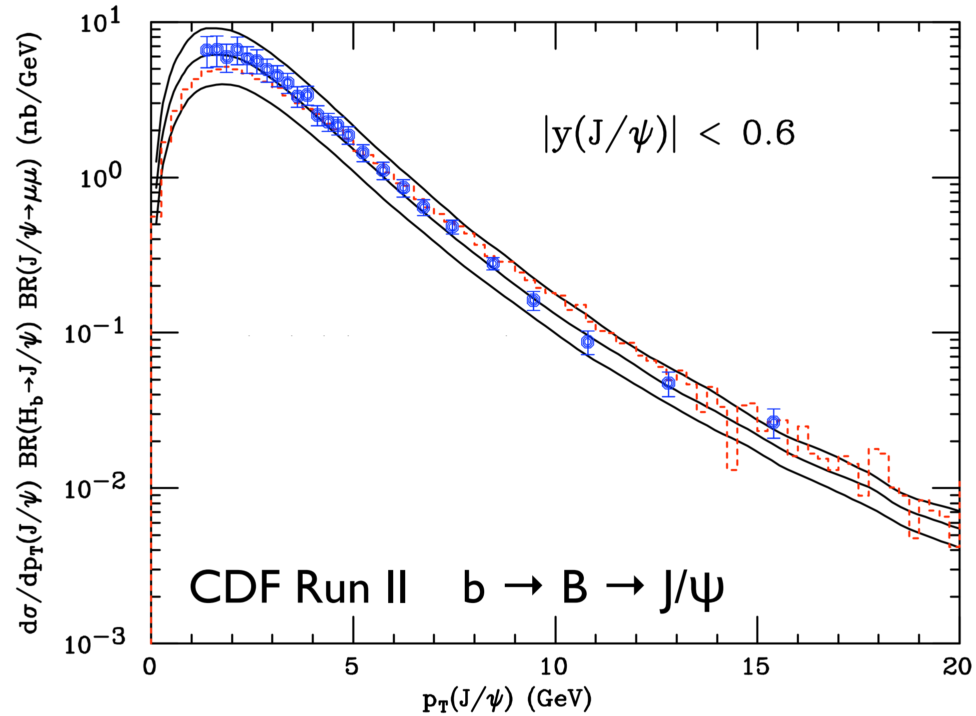
Bottom production @: Run I vs Run 2

'Before'



'Factor of 3' excess

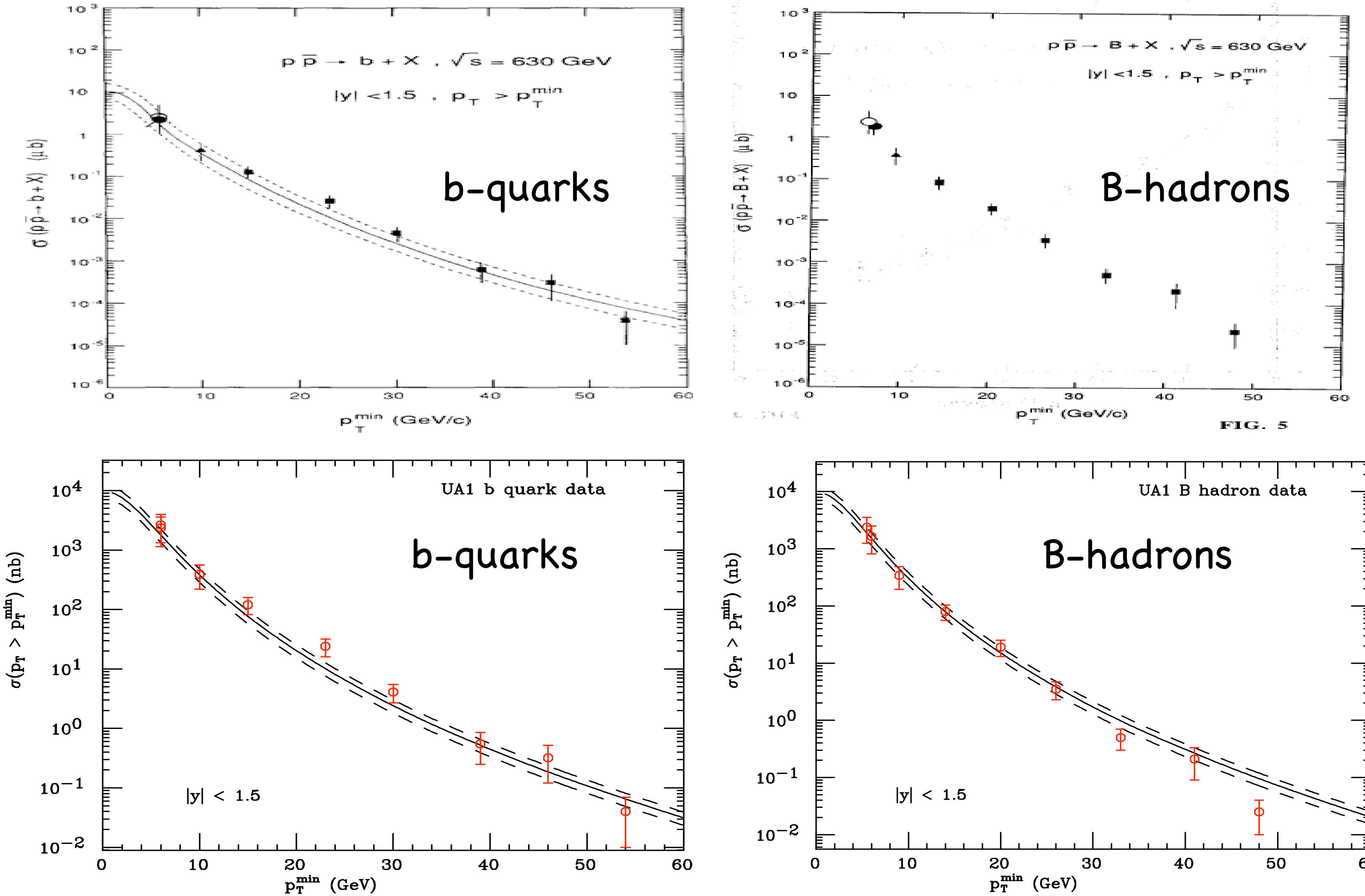
'After'



Perfect agreement

Key improvement:
b → B non-perturbative fragmentation properly extracted from LEP data within the FONLL framework

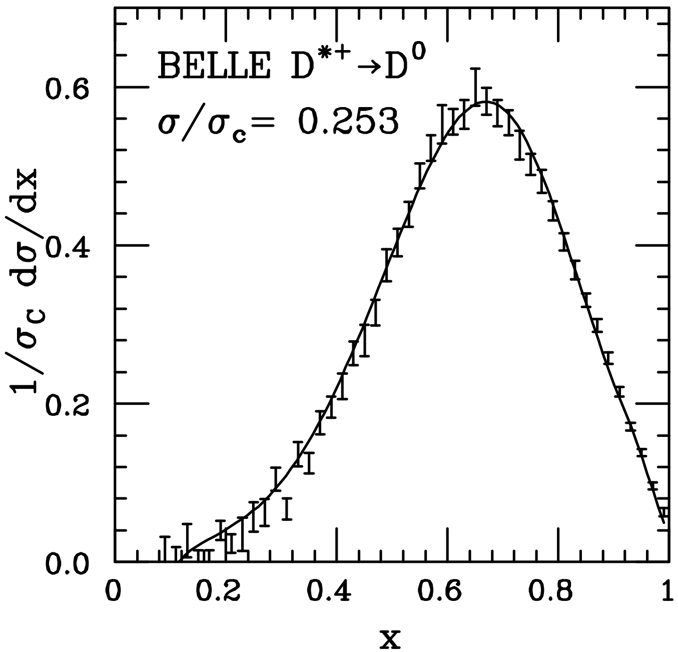
What about the old UA1 data?

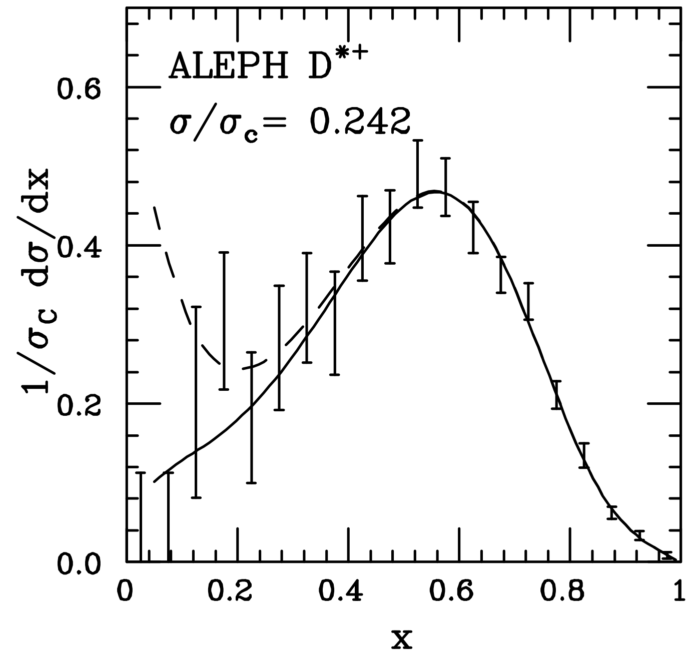


No artificial inflation of theoretical prediction to 'fit' the tevatron data

Charm

D* fragmentation from BELLE and ALEPH



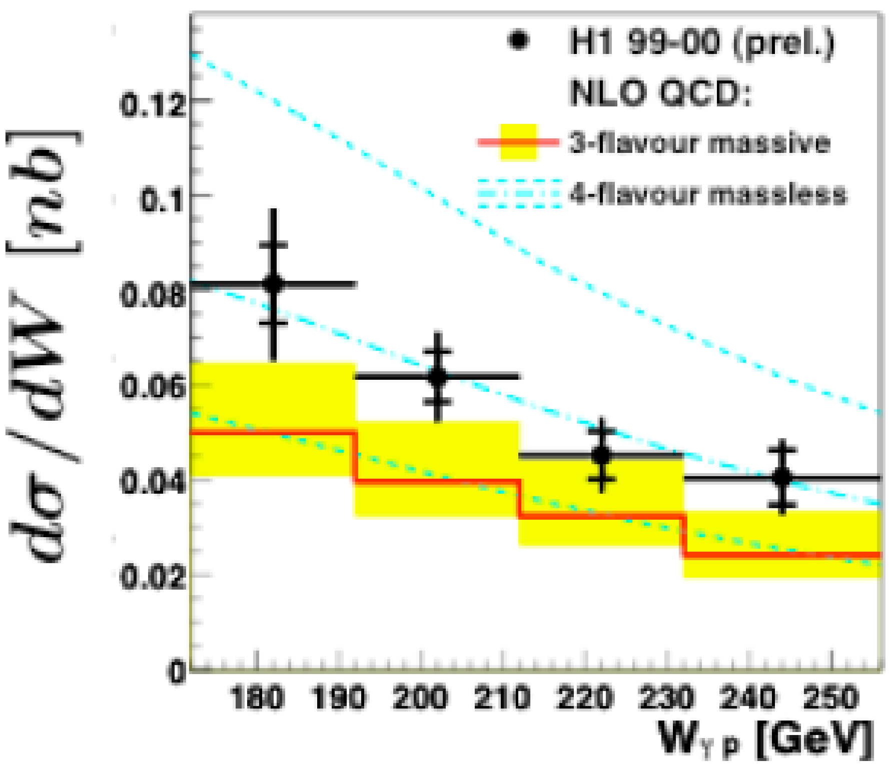


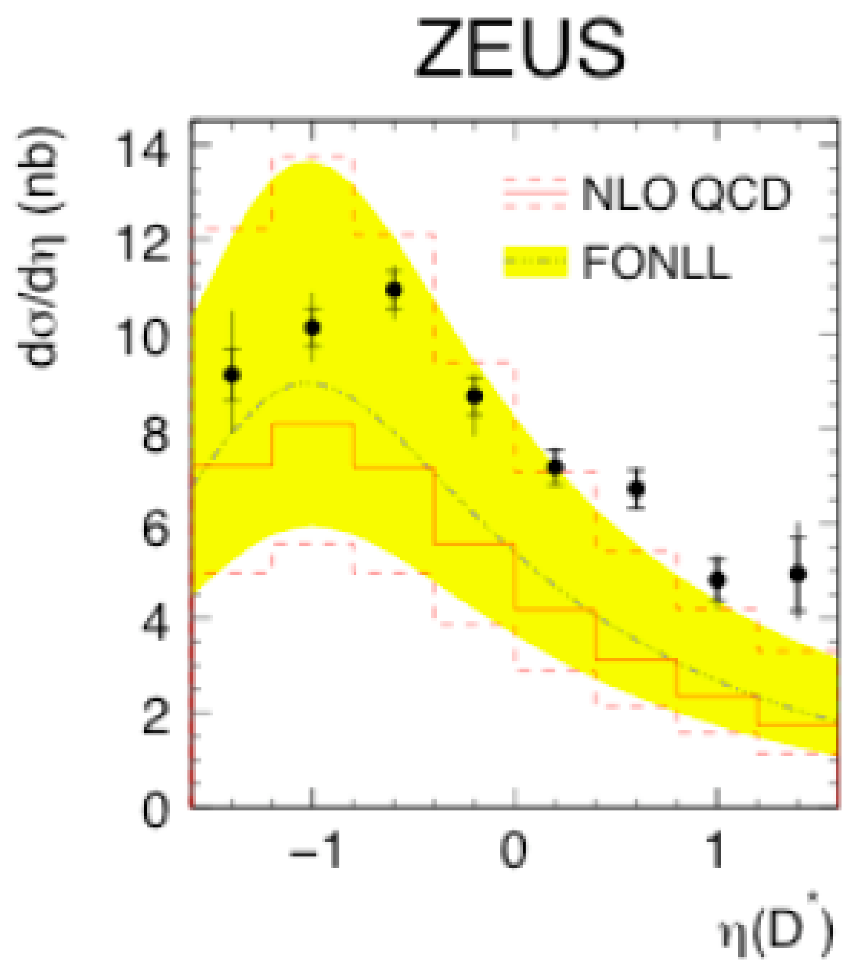
These curves contain two contributions:
a perturbative one convoluted with a non-perturbative term

The experimentally observed fragmentation is different at the two machines (of course!), but thanks to collinear resummation **the extracted non-perturbative contributions coincide to within about 10%**

==> not much uncertainty on the hadronic production rates, once fragmentation is properly implemented

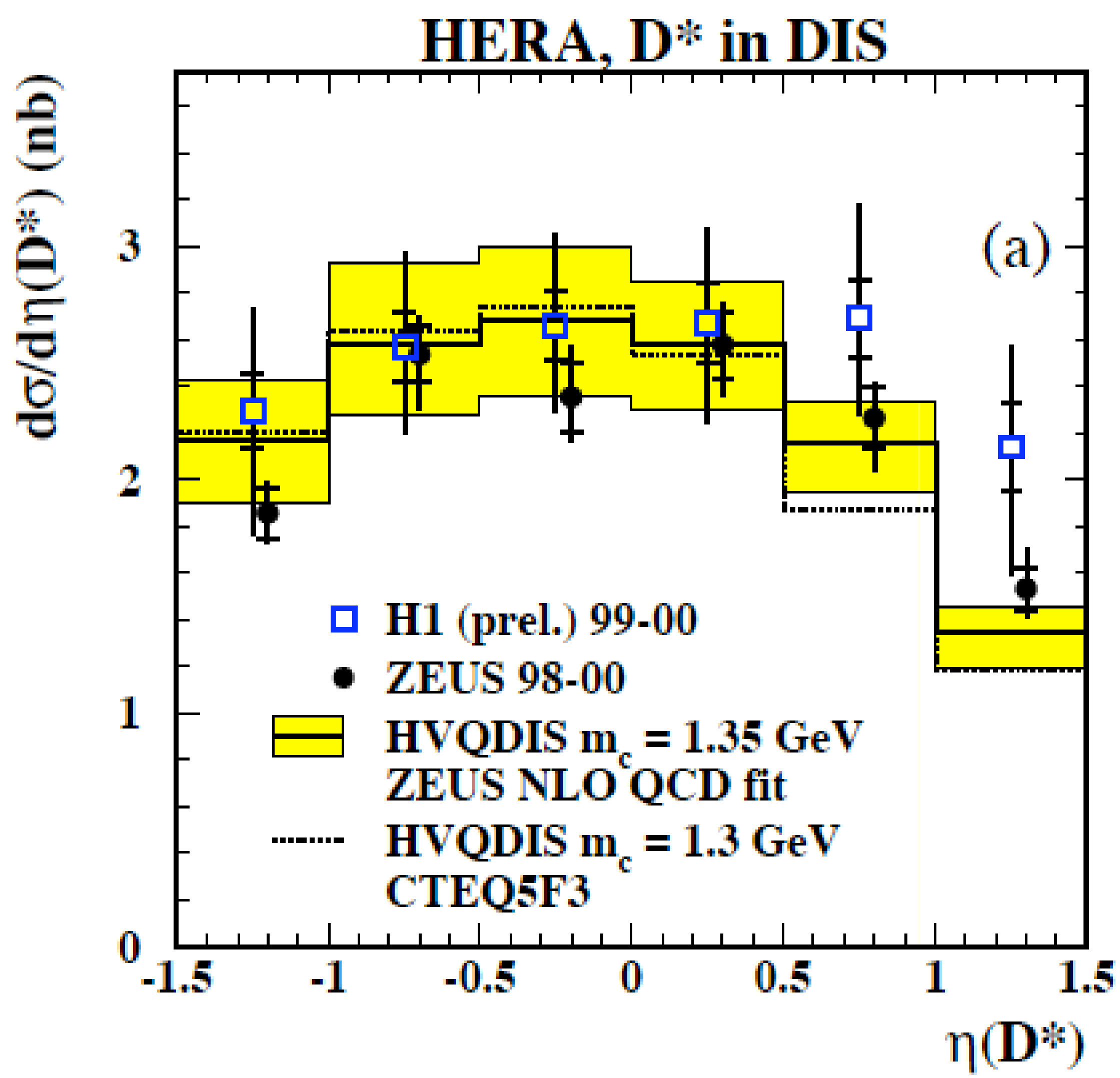
Charm photoproduction @ HERA



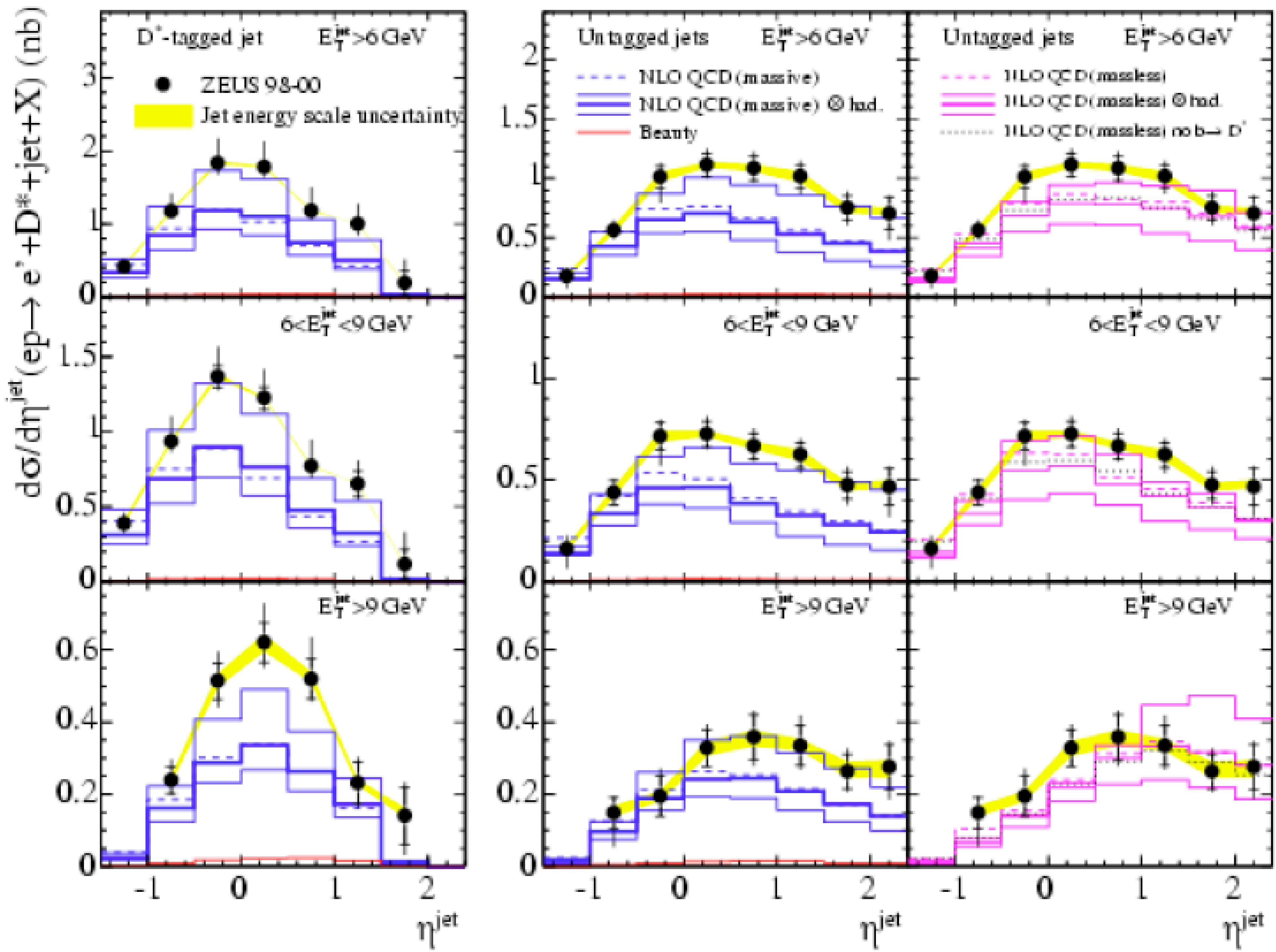


At least 50% theoretical uncertainty. Expt. data more precise

Charm production in DIS @ HERA



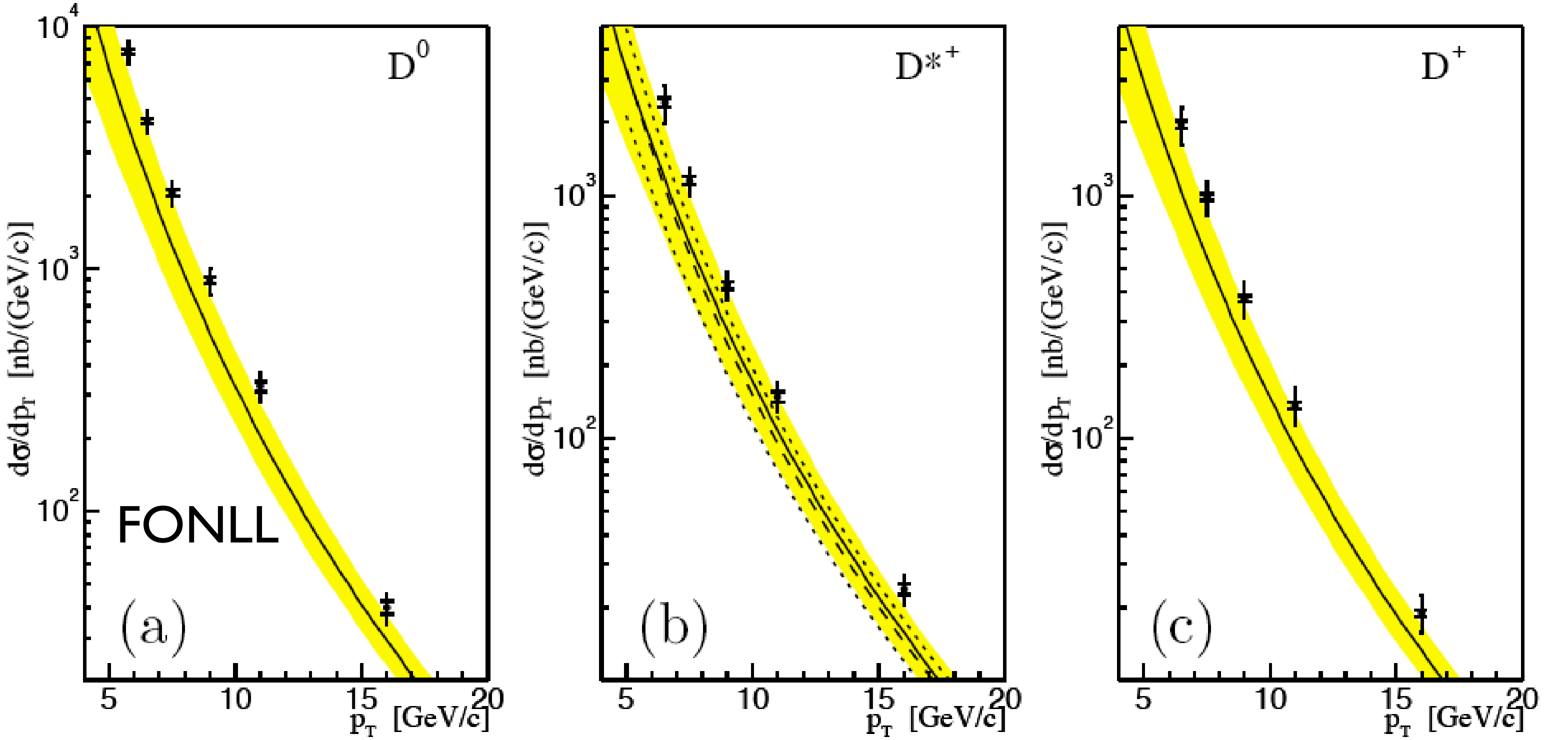
D* + jet @ HERA



D*-tagged jet
$E_T^{jet}>6$ GeV
ZEUS 98-00
Jet energy scale uncertainty
Untagged jets
NLO QCD (massive)
NLO QCD (massive) ⊗ had.
Beauty
NLO QCD (massless)
NLO QCD (massless) ⊗ had.
NLO QCD (massless) no b→ D*
$6<E_T^{jet}<9$ GeV
$E_T^{jet}>9$ GeV
$d\sigma/d\eta^{jet}(ep \to e' + D^* + jet + X)$ (nb)
η^{jet}

Charm production @ Tevatron Run 2

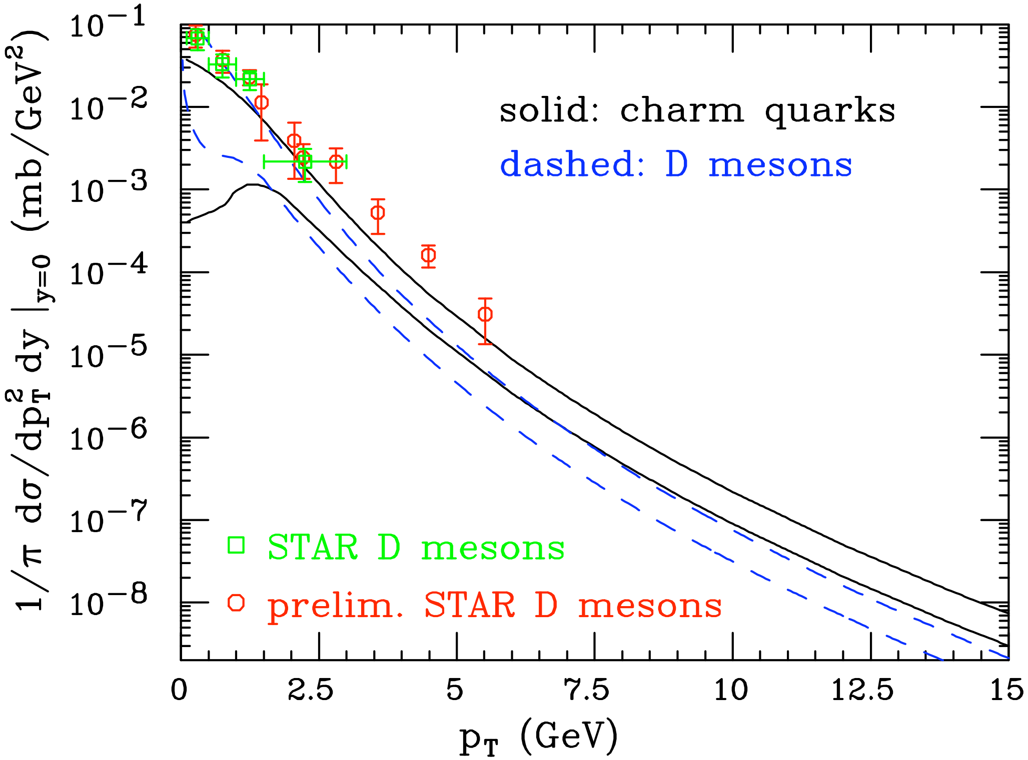
CDF Run II   c → D data   [PRL 91:241804,2003]

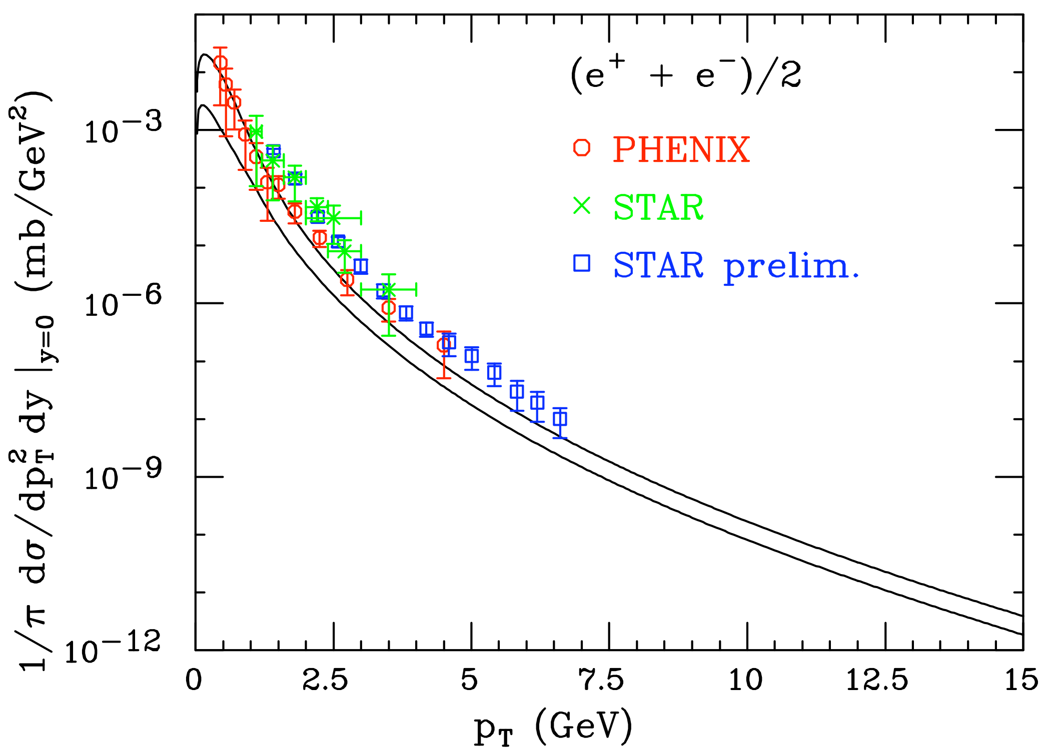


The non-perturbative charm fragmentation needed to describe the c → D hadronization has been extracted from moments of ALEPH data at LEP.

Charm and bottom production @ RHIC

The very same FONLL formalism + NP FF can be applied at RHIC





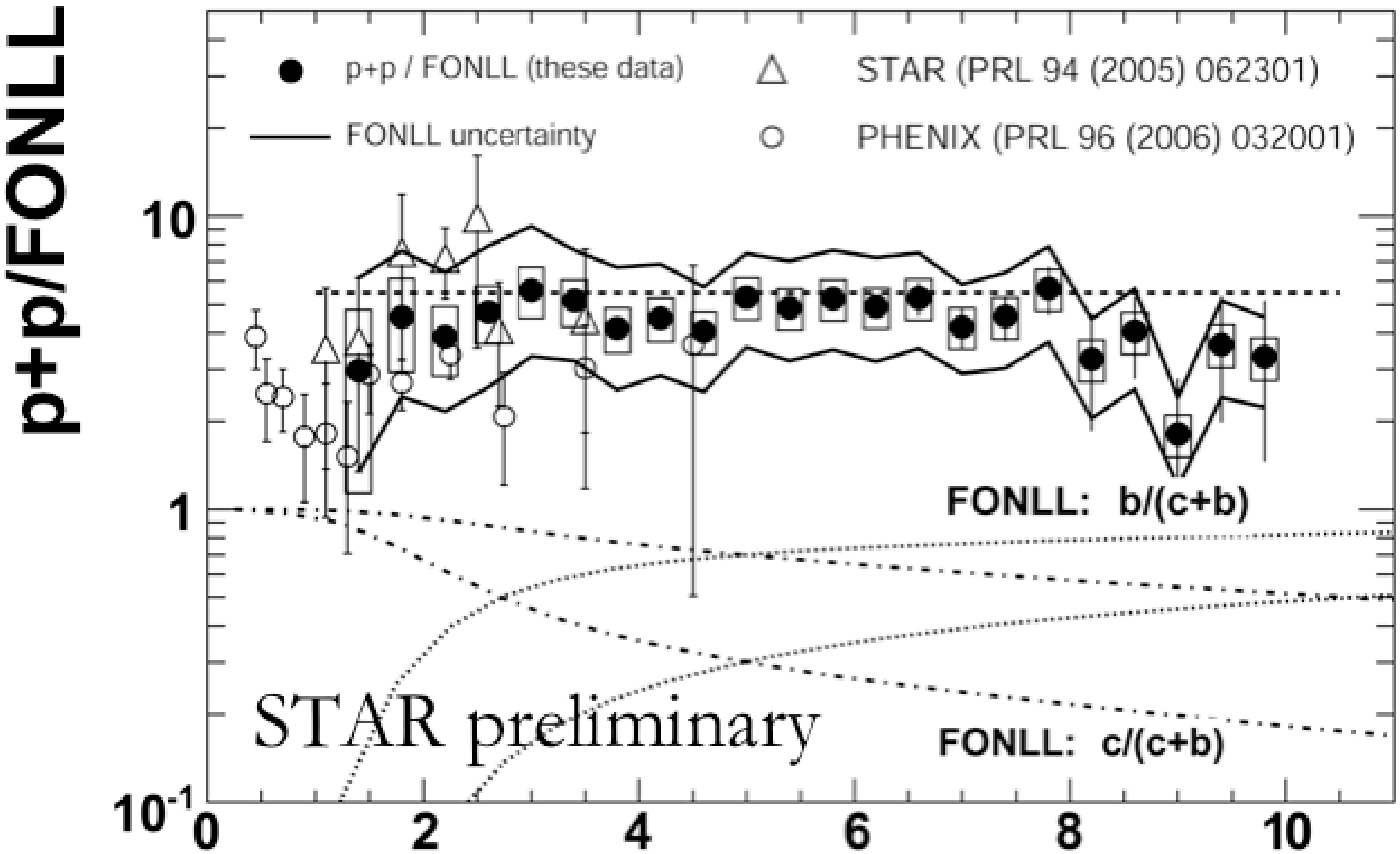
Fair agreement. In line with other measurements.

Note, though, the large theoretical uncertainties at low transverse momentum, especially for charm.

But, what happens with STAR preliminary measurements at large p_T?

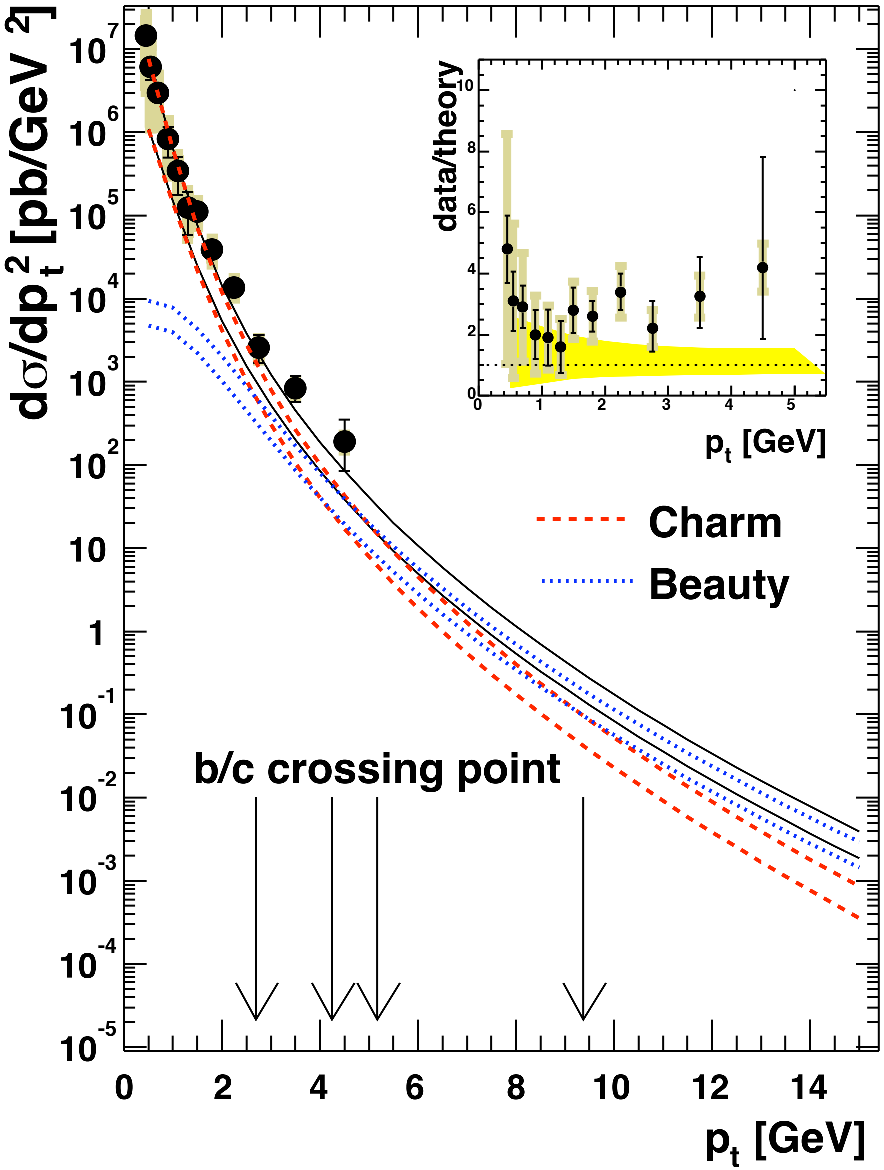
Charm and bottom production @ RHIC

Plot stolen from Thomas Ullrich's talk



A factor of five excess would seem to be a bit too large, if compared to measurements in other experiments (though it's a lot less when including both theoretical and experimental uncertainties)

Relative Charm and Bottom contributions @ RHIC

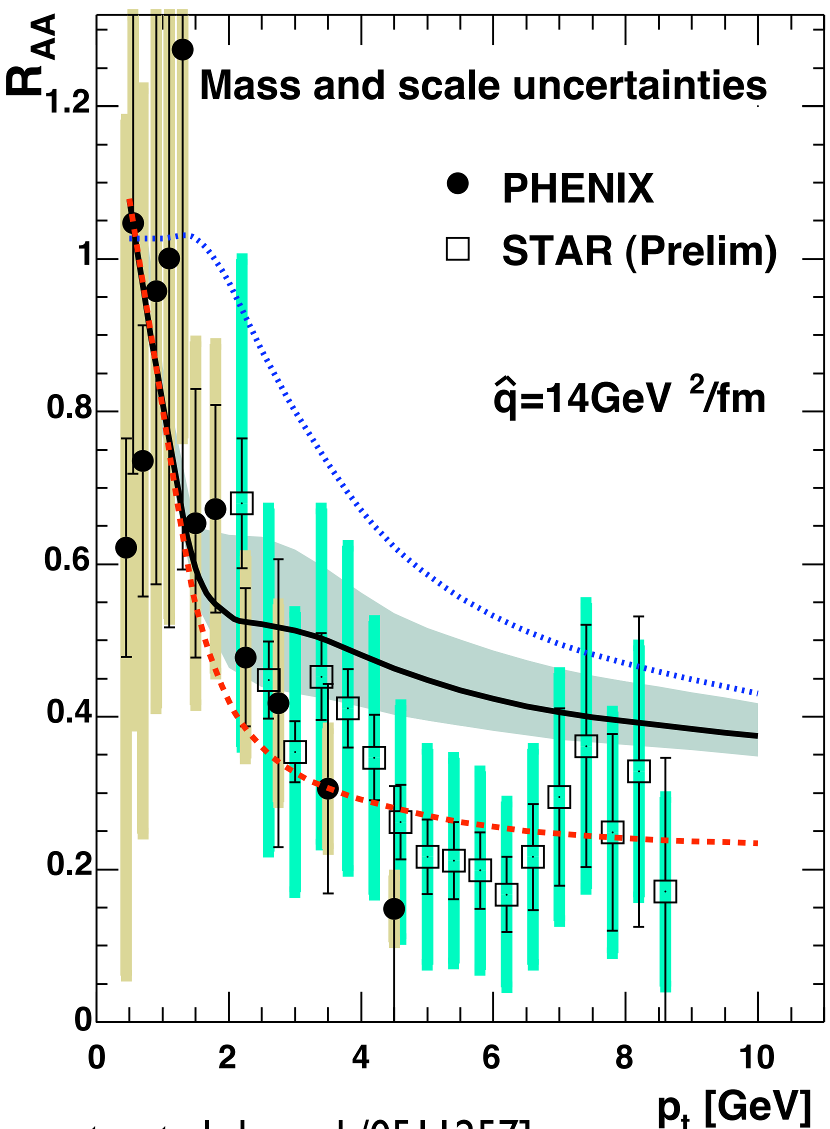


The slope of the charm and bottom contribution is fairly similar: the crossing point easily moves, though the relative contributions are less affected by uncertainties

NB. Especially for bottom the transverse momentum is small: all the uncertainties previously mentioned can apply

R_AA for Charm and bottom @ RHIC

The charm and bottom spectra translate into R_AA via the application of quenching weights



[Armesto et al., hep-ph/0511257]

The uncertainty on the charm and bottom relative contribution reflects on an uncertainty of order 0.1 on R_AA

R_AA looks too high. However, remember the very large perturbative uncertainty on charm: the NNLO prediction could be quite larger.

Observation: if you normalize charm to the data R_AA comes out about right

Conclusions

- Heavy quark phenomenology is mature and has the tools to produce predictions in many **realistic** situations. These predictions can include all the available knowledge for calculating heavy quark production in QCD. Since they are implemented in a rigorous framework, it is usually possible to also provide a (more or less reliable) estimate of the **theoretical uncertainty**

- Most predictions seem to agree well with Tevatron and HERA data for charm and bottom production. They should provide a solid benchmark for pp collisions at RHIC. The apparent STAR charm excess looks puzzling. Whatever the case, uncertainties being large, normalization to a pp baseline better be done using data or a reliable extrapolation

- Final note: given the size of intrinsic pQCD uncertainty, it is very unlikely that effects of the order of a few (tens of) percent will ever be visible just by comparing to the absolute value of the cross sections